

Supplementary Information for
**Kohn-Sham Calculations of NMR shifts for paramagnetic 3d metal
complexes: Protocols, impact of the delocalization error, and analysis of the
curious amide proton shifts of a high-spin iron(II) macrocycle complex**

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1 Optimized Geometries of the Complexes

Table S1: Optimized structure of nickelocene in xyz format.

Atoms	X	Y	Z
Ni	-0.000003	-0.000121	0.000040
H	-0.770480	2.166738	1.827595
C	-0.407044	1.144482	1.830829
H	-2.298940	-0.063179	1.827493
C	-1.214414	-0.033433	1.830800
H	-0.650459	-2.205939	1.827392
C	-0.343646	-1.165285	1.830689
H	1.896785	-1.300293	1.827359
C	1.001898	-0.686889	1.830656
H	1.822623	1.402164	1.827470
C	0.962708	0.740628	1.830744
H	-0.650291	-2.205705	-1.827545
C	-0.343476	-1.165061	-1.830670
H	1.896964	-1.300107	-1.827836
C	1.002079	-0.686697	-1.830886
H	1.822819	1.402365	-1.827674
C	0.962921	0.740805	-1.830825
H	-0.770254	2.166953	-1.827314
C	-0.406806	1.144707	-1.830585
C	-1.214228	-0.033190	-1.830484
H	-2.298756	-0.062941	-1.827245

Table S2: Optimized structure of vanadocene in xyz format.

Atoms	X	Y	Z
V	0.000062	-0.000040	-0.000001
H	-0.769978	2.165578	1.940890
C	-0.406403	1.142948	1.934539
H	-2.297636	-0.063139	1.940770
C	-1.212706	-0.033374	1.934474
H	-0.650066	-2.204748	1.940787
C	-0.343115	-1.163720	1.934483
H	1.895845	-1.299611	1.940919
C	1.000623	-0.685986	1.934553
H	1.821742	1.401397	1.940985
C	0.961510	0.739612	1.934589
H	-0.650032	-2.204537	-1.941030
C	-0.343080	-1.163509	-1.934621
H	1.895883	-1.299390	-1.941025
C	1.000656	-0.685770	-1.934614
H	1.821766	1.401617	-1.940793
C	0.961537	0.739827	-1.934494
H	-0.769952	2.165791	-1.940665
C	-0.406375	1.143159	-1.934428
C	-1.212675	-0.033167	-1.934506
H	-2.297606	-0.062936	-1.940808

Table S3: Optimized structure of manganocene in xyz format.

Atoms	X	Y	Z
Mn	0.000020	-0.000202	0.000004
H	-0.769812	2.165365	2.090540
C	-0.406250	1.142520	2.073141
H	-2.297449	-0.062954	2.090595
C	-1.212318	-0.033271	2.073175
H	-0.650250	-2.204428	2.090507
C	-0.343167	-1.163234	2.073110
H	1.895426	-1.299594	2.090396
C	1.000082	-0.685795	2.073034
H	1.821523	1.401098	2.090409
C	0.961089	0.739248	2.073051
H	-0.649687	-2.204301	-2.090657
C	-0.342757	-1.163062	-2.073177
H	1.895846	-1.299064	-2.090829
C	1.000410	-0.685404	-2.073291
H	1.821529	1.401597	-2.090535
C	0.961196	0.739618	-2.073146
H	-0.769913	2.165485	-2.090178
C	-0.406198	1.142691	-2.072937
C	-1.212097	-0.033231	-2.072958
H	-2.297224	-0.063081	-2.090254

Table S4: Optimized structure of CrL¹ in xyz format.

Atoms	X	Y	Z
N	-0.541235	3.367822	-0.609098
C	-1.082683	2.156037	-0.496590
C	-2.464895	1.958638	-0.310101
C	-3.308614	3.046997	-0.238377
C	-2.771923	4.354551	-0.353648
C	-1.363474	4.475211	-0.540779
C	-3.545097	5.542648	-0.294652
C	-2.939806	6.776343	-0.416265
C	-1.541692	6.882016	-0.601433
C	-0.750028	5.749178	-0.664735
C	0.721415	5.737931	-0.855264
C	1.386969	5.559336	-2.113223
C	2.777504	5.343689	-1.828433
C	1.687090	5.638927	0.200707
C	0.770314	5.633713	-3.476264
H	1.041150	6.579420	-3.971542
H	-0.324157	5.587696	-3.422452
H	1.114294	4.806743	-4.110715
C	3.836986	5.154345	-2.869683
H	4.080399	6.116918	-3.346418
H	3.500336	4.462549	-3.652200
H	4.760371	4.750638	-2.439943
C	4.252444	5.264500	0.333484
C	1.437420	5.810761	1.667611
H	1.816391	6.785764	2.012210
H	1.939648	5.026142	2.248019
H	0.365862	5.769960	1.897768
H	-2.844830	0.942838	-0.225354
H	-4.381337	2.917450	-0.094479
C	2.960993	5.392395	-0.413746
H	5.039391	4.824823	-0.289165
H	4.132402	4.629885	1.220671
H	4.600778	6.254845	0.666560
H	-0.387945	1.321452	-0.557823
H	-4.622417	5.464522	-0.152035
H	-3.540767	7.682829	-0.369872
H	-1.080743	7.864225	-0.695467
Cr	1.482279	3.697201	-0.883611
Cl	1.725448	2.242327	-2.610149
Cl	2.171229	2.360135	0.817666

Table S5: Optimized structure of CrL² in xyz format.

Atoms	X	Y	Z
N	-0.494607	3.324928	-0.588286
C	-0.998783	2.098338	-0.459331
C	-2.373889	1.859109	-0.270970
C	-3.252278	2.920397	-0.214511
C	-2.757421	4.242343	-0.347282
C	-1.353032	4.405762	-0.535383
C	-3.569427	5.405022	-0.304649
C	-3.005351	6.656253	-0.442512
C	-1.611295	6.804822	-0.628513
C	-0.782961	5.697802	-0.676212
C	0.687511	5.734955	-0.866201
C	1.359701	5.566074	-2.121872
C	2.757549	5.408585	-1.834198
C	1.655498	5.687860	0.191075
C	0.740305	5.615462	-3.484682
H	0.956493	6.580220	-3.970191
H	-0.349653	5.505893	-3.432271
H	1.131140	4.815425	-4.126248
C	3.829524	5.265001	-2.869703
H	4.071153	6.247345	-3.305723
H	3.507915	4.601248	-3.681775
H	4.750859	4.851679	-2.444671
C	4.237729	5.433025	0.322048
C	1.397310	5.885898	1.653083
H	1.715876	6.892610	1.966548
H	1.946919	5.151105	2.255108
H	0.330575	5.786183	1.887384
H	-2.720630	0.832748	-0.172674
H	-4.320447	2.758612	-0.069467
C	2.938364	5.482999	-0.420355
H	5.028118	4.965353	-0.275368
H	4.138914	4.861528	1.253226
H	4.568342	6.451928	0.579013
H	-0.278917	1.284507	-0.508561
H	-4.643660	5.292978	-0.161483
H	-3.635717	7.543063	-0.408555
H	-1.182456	7.800155	-0.735640
Cr	1.521571	3.723350	-0.866971
Br	1.850350	2.149987	-2.691579
Br	2.318279	2.342846	0.969533

Table S6: Optimized structure of $(\text{FeL}^3)^{2+}$ in xyz format.

Atoms	X	Y	Z
Fe	0.000961	-0.020597	-0.808693
N	-1.302312	-1.054273	0.683291
N	1.588406	-0.617035	0.679846
N	-0.245535	1.648257	0.670449
C	-1.241359	1.245226	1.708955
H	-0.702786	0.988619	2.628590
H	-1.898749	2.085408	1.974421
C	-2.110516	0.066779	1.249601
H	-2.731580	-0.275850	2.095141
H	-2.795535	0.401961	0.457637
C	-0.438471	-1.724995	1.701965
H	-0.482430	-1.143864	2.630546
H	-0.830118	-2.720154	1.956455
C	1.016766	-1.879492	1.236633
H	1.069907	-2.634210	0.438876
H	1.623214	-2.253450	2.079794
C	1.734192	0.470821	1.692543
H	2.790994	0.632414	1.948046
H	1.251538	0.149071	2.622886
C	1.138527	1.799755	1.208396
H	1.756616	2.206159	0.394642
H	1.167026	2.529468	2.036295
C	2.825605	-0.885366	-0.077525
H	3.495114	-1.596916	0.435925
H	3.380274	0.056037	-0.201526
C	-2.152907	-1.990075	-0.076335
H	-1.600783	-2.928515	-0.230716
H	-3.087762	-2.240388	0.454124
C	-0.655236	2.847396	-0.090060
H	-0.379185	3.784746	0.422083
H	-1.749883	2.841946	-0.196824
C	2.453472	-1.385076	-1.474880
C	-2.446107	-1.403120	-1.461978
C	-0.067744	2.789549	-1.503230
O	0.284361	1.691177	-1.987572
O	-1.719901	-0.493995	-1.925485
O	1.293980	-1.188578	-1.911539
N	-3.472047	-1.908196	-2.147528
H	-3.649468	-1.580143	-3.093595
H	-4.071640	-2.634497	-1.771027

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Table S6 – continued from previous page

Atoms	X	Y	Z
N	3.388687	-1.998569	-2.199416
H	3.177097	-2.283933	-3.152246
H	4.323246	-2.169281	-1.844191
N	0.018862	3.930973	-2.190322
H	-0.257458	4.823609	-1.796483
H	0.338372	3.909337	-3.155296

Table S7: Optimized structure of $(\text{FeL}^4)^{2+}$ in xyz format.

Atoms	X	Y	Z
Fe	-0.327467	0.062759	0.114238
N	-1.007365	1.145435	2.016980
N	-2.219707	1.121341	-0.557439
N	-1.964181	-1.291112	0.941850
C	-2.118005	2.104493	1.718464
H	-1.949260	3.058800	2.241046
H	-3.047435	1.692569	2.131092
H	-3.233316	2.918483	0.055038
C	-2.283813	2.380527	0.221250
H	-1.474006	3.027418	-0.136002
H	-4.002831	0.683051	0.492270
C	-3.425041	0.260690	-0.339284
H	-4.086287	0.296356	-1.218827
C	-3.068480	-1.199517	-0.045395
H	-2.730140	-1.698033	-0.961527
H	-3.969693	-1.732102	0.303691
H	-2.515881	-1.767391	2.958169
C	-2.400362	-0.881857	2.314658
H	-3.396335	-0.428146	2.237315
C	-1.424334	0.095190	2.975766
H	-0.519602	-0.433633	3.297301
H	-1.892605	0.526455	3.877292
H	-2.864206	1.735346	-2.509462
C	-1.964557	1.362594	-1.993101
H	-1.204985	2.156494	-2.058061
H	0.906654	1.073617	2.837893
C	0.219014	1.842002	2.453921
H	0.015226	2.540371	3.282331
H	-1.221808	-2.932959	-0.110202
C	-1.326864	-2.624527	0.941146
H	-1.963397	-3.376965	1.434953
C	-1.457482	0.119148	-2.677611
C	-0.356499	-2.086403	-3.944450
C	-1.921047	-0.254496	-3.935065
N	-0.484326	-0.588587	-2.041231
C	0.075412	-1.657829	-2.654619
C	-1.381231	-1.360955	-4.572105
H	-2.704360	0.326728	-4.418545
H	-1.742104	-1.663032	-5.555006
C	0.869687	2.573583	1.312143

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Table S7 – continued from previous page

Atoms	X	Y	Z
C	2.230772	3.784659	-0.770719
N	1.000566	1.896862	0.137017
C	1.375110	3.859168	1.475517
C	2.049340	4.478632	0.435053
C	1.686182	2.471418	-0.881183
H	1.245239	4.373673	2.426148
H	2.445321	5.486855	0.552976
C	0.029315	-2.586653	1.594569
C	2.604718	-2.564868	2.603579
C	0.441624	-3.606232	2.447652
C	2.119857	-1.543056	1.734889
C	1.727395	-3.599307	2.963969
H	-0.246531	-4.409978	2.704057
H	2.059907	-4.392087	3.633562
N	0.851535	-1.555125	1.260858
C	1.200184	-2.393830	-1.995064
H	2.109507	-2.349984	-2.615892
H	0.958507	-3.459336	-1.859249
H	1.435619	-1.971660	-1.015204
C	1.929092	1.709382	-2.147859
H	1.513662	2.234277	-3.022063
H	1.488352	0.711300	-2.109168
H	3.010282	1.595456	-2.327742
C	3.068225	-0.464432	1.310947
H	3.948331	-0.902577	0.814901
H	3.443542	0.110535	2.172804
H	2.592307	0.236736	0.622522
N	2.879177	4.362771	-1.830831
H	3.392291	5.222443	-1.680834
H	3.195288	3.798864	-2.607656
N	0.190164	-3.196377	-4.530649
H	1.052684	-3.590776	-4.181730
H	-0.022596	-3.397863	-5.499537
N	3.904371	-2.553559	3.036774
H	4.465321	-1.716598	2.958752
H	4.188460	-3.204536	3.757957

Table S8: Optimized saddled structure of FeL⁵ in xyz format.

Atoms	X	Y	Z
C	0.679199	4.249024	0.256491
C	0.679199	-4.249024	0.256491
C	-0.679199	4.249024	0.256491
C	-0.679199	-4.249024	0.256491
C	1.089998	2.857952	0.096028
C	1.089998	-2.857952	0.096028
C	-1.089998	2.857952	0.096028
C	-1.089998	-2.857952	0.096028
C	2.443082	2.461102	0.037805
C	2.443082	-2.461102	0.037805
C	-2.443082	2.461102	0.037805
C	-2.443082	-2.461102	0.037805
C	2.894146	1.131775	-0.007140
C	2.894146	-1.131775	-0.007140
C	-2.894146	1.131775	-0.007140
C	-2.894146	-1.131775	-0.007140
C	3.490736	3.523740	0.012453
C	3.490736	-3.523740	0.012453
C	-3.490736	3.523740	0.012453
C	-3.490736	-3.523740	0.012453
C	3.547742	4.444475	-1.047872
C	3.547742	-4.444475	-1.047872
C	-3.547742	4.444475	-1.047872
C	-3.547742	-4.444475	-1.047872
C	4.248924	0.686443	-0.157047
C	4.248924	-0.686443	-0.157047
C	-4.248924	0.686443	-0.157047
C	-4.248924	-0.686443	-0.157047
C	4.440249	3.623668	1.043446
C	4.440249	-3.623668	1.043446
C	-4.440249	3.623668	1.043446
C	-4.440249	-3.623668	1.043446
C	4.527172	5.439967	-1.076401
C	4.527172	-5.439967	-1.076401
C	-4.527172	5.439967	-1.076401
C	-4.527172	-5.439967	-1.076401
C	5.421266	4.618038	1.016352
C	5.421266	-4.618038	1.016352
C	-5.421266	4.618038	1.016352
C	-5.421266	-4.618038	1.016352

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Table S8 – continued from previous page

Atoms	X	Y	Z
C	5.468268	5.530277	-0.044224
C	5.468268	-5.530277	-0.044224
C	-5.468268	5.530277	-0.044224
C	-5.468268	-5.530277	-0.044224
Cl	-0.000002	-0.000001	-2.640890
Fe	0.000002	0.000000	-0.445371
H	1.343848	5.097652	0.379914
H	1.343848	-5.097652	0.379914
H	-1.343848	5.097652	0.379914
H	-1.343848	-5.097652	0.379914
H	2.815246	4.368409	-1.852958
H	2.815246	-4.368409	-1.852958
H	-2.815246	4.368409	-1.852958
H	-2.815246	-4.368409	-1.852958
H	4.396294	2.916629	1.873596
H	4.396294	-2.916629	1.873596
H	-4.396294	2.916629	1.873596
H	-4.396294	-2.916629	1.873596
H	4.558014	6.143299	-1.910233
H	4.558014	-6.143299	-1.910233
H	-4.558014	6.143299	-1.910233
H	-4.558014	-6.143299	-1.910233
H	5.101930	1.345123	-0.271962
H	5.101930	-1.345123	-0.271962
H	-5.101930	1.345123	-0.271962
H	-5.101930	-1.345123	-0.271962
H	6.146049	4.684070	1.829397
H	6.146049	-4.684070	1.829397
H	-6.146049	4.684070	1.829397
H	-6.146049	-4.684070	1.829397
H	6.233498	6.307376	-0.066034
H	6.233498	-6.307376	-0.066034
H	-6.233498	6.307376	-0.066034
H	-6.233498	-6.307376	-0.066034
N	0.000000	2.026225	0.022936
N	0.000000	-2.026225	0.022936
N	2.111559	0.000000	0.070721
N	-2.111559	0.000000	0.070721

Table S9: Optimized planar structure of FeL⁵ in xyz format.

Atoms	X	Y	Z
C	0.679688	4.209082	0.188841
C	0.682735	-4.208859	0.184514
C	-0.682687	4.208930	0.184843
C	-0.679638	-4.209016	0.188609
C	1.102732	2.850246	-0.034027
C	1.104087	-2.849783	-0.039994
C	-1.104063	2.849866	-0.039708
C	-1.102707	-2.850172	-0.034167
C	2.443394	2.441598	-0.083321
C	2.444401	-2.440486	-0.093505
C	-2.444382	2.440574	-0.093204
C	-2.443376	-2.441528	-0.083362
C	2.856031	1.104229	-0.165044
C	2.856540	-1.102756	-0.170762
C	-2.856511	1.102841	-0.170557
C	-2.856007	-1.104149	-0.164986
C	3.496194	3.498106	-0.007613
C	3.497277	-3.497377	-0.025393
C	-3.497290	3.497436	-0.025097
C	-3.496150	-3.498065	-0.007704
C	3.634515	4.448306	-1.030974
C	3.632594	-4.442454	-1.053847
C	-3.632447	4.442657	-1.053443
C	-3.634274	-4.448351	-1.031015
C	4.230235	0.682543	-0.257401
C	4.230534	-0.680042	-0.261294
C	-4.230501	0.680130	-0.261168
C	-4.230204	-0.682456	-0.257348
C	4.362503	3.568073	1.094718
C	4.365839	-3.573420	1.074692
C	-4.366130	3.573245	1.074790
C	-4.362595	-3.568033	1.094525
C	4.614117	5.440280	-0.955427
C	4.611590	-5.435523	-0.985416
C	-4.611569	5.435607	-0.985120
C	-4.613787	-5.440411	-0.955515
C	5.339183	4.562295	1.173394
C	5.341766	-4.568881	1.146346
C	-5.342207	4.568570	1.146324
C	-5.339205	-4.562334	1.173145

Continued on next page

Table S9 – continued from previous page

Atoms	X	Y	Z
C	5.469011	5.501703	0.147649
C	5.468643	-5.503219	0.115590
C	-5.468931	5.503034	0.115663
C	-5.468819	-5.501828	0.147454
Cl	-0.000078	0.000162	-2.878040
Fe	-0.000004	0.000065	-0.681275
H	1.341910	5.049686	0.356176
H	1.346189	-5.049282	0.347874
H	-1.346124	5.049352	0.348290
H	-1.341843	-5.049626	0.355960
H	2.972110	4.397623	-1.894596
H	2.968211	-4.386961	-1.915650
H	-2.967855	4.387348	-1.915096
H	-2.971768	-4.397671	-1.894563
H	4.256234	2.841629	1.899959
H	4.261841	-2.850933	1.883779
H	-4.262254	2.850657	1.883802
H	-4.256483	-2.841534	1.899735
H	4.710880	6.164488	-1.763429
H	4.706096	-6.155733	-1.797241
H	-4.705947	6.155921	-1.796867
H	-4.710366	-6.164694	-1.763467
H	5.083793	1.345966	-0.323787
H	5.084402	-1.342692	-0.331425
H	-5.084363	1.342784	-0.331315
H	-5.083758	-1.345876	-0.323812
H	5.996096	4.605234	2.041459
H	6.000365	-4.616727	2.012855
H	-6.001066	4.616211	2.012657
H	-5.996234	-4.605281	2.041129
H	6.231767	6.277425	0.208026
H	6.230748	-6.279979	0.170421
H	-6.231159	6.279679	0.170395
H	-6.231518	-6.277612	0.207792
N	-0.000253	2.029907	-0.157119
N	0.000266	-2.029821	-0.157288
N	2.026509	0.000500	-0.142161
N	-2.026482	-0.000420	-0.142014

2 Basis Set Dependence of PNMR Shifts of Metallocenes

Table S10: Total Shielding Constants for Metallocenes and TMS (ppm) calculated with a range of STO basis sets and the PBE0 functional ^a

		DZ-DZ ^b	DZ-TZ2P	DZ-QZ4P	TZ2P-DZ	TZ2P-TZ2P	TZ2P-QZ4P
Ni	H	395.69	316.67	298.25	386.58	311.27	293.71
	C	-1000.85	-1410.89	-1336.71	-1020.52	-1414.78	-1341.98
V	H	-400.71	-358.96	-345.98	-394.11	-352.72	-340.88
	C	498.41	648.35	689.94	520.94	646.52	695.06
Mn	H	71.62	43.99	40.00	72.37	44.01	38.14
	C	-1171.72	-1360.44	-1233.48	-1155.32	-1360.10	-1229.75
TMS	H	32.60	31.05	30.88	32.23	30.90	30.79
	C	205.15	186.85	183.07	202.45	187.00	181.69
		QZ4P-DZ	QZ4P-TZ2P	QZ4P-QZ4P			
Ni	H	370.45	311.10	292.65			
	C	-1050.43	-1415.62	-1344.47			
V	H	-383.25	-346.70	-344.07			
	C	558.96	620.39	710.45			
Mn	H	62.00	48.92	34.63			
	C	-1170.21	-1362.82	-1217.00			
TMS	H	32.19	30.91	30.80			
	C	201.05	185.69	181.72			

^a: $T = 298\text{K}$ for Ni and V. Shieldings and shifts for MnCp_2 were calculated at 390K . ^b: The first basis set listed corresponds to the metal or Silicon atom, and the second basis set listed was used for the Carbon and Hydrogen atoms.

Table S11: Chemical shifts for Metallocenes (ppm) calculated with a range of STO basis sets and the PBE0 functional ^a

		DZ-DZ ^b	DZ-TZ2P	DZ-QZ4P	TZ2P-DZ	TZ2P-TZ2P	TZ2P-QZ4P
Ni	H	-363.09	-285.62	-267.37	-354.35	-280.37	-262.92
	C	1206.00	1597.74	1519.78	1222.97	1601.78	1523.67
V	H	433.31	390.01	376.86	426.34	383.62	371.67
	C	-293.26	-461.50	-506.87	-318.49	-459.52	-513.37
Mn	H	-39.01	-12.94	-9.12	-40.14	-13.11	-7.35
	C	1376.87	1547.29	1416.55	1357.77	1547.10	1411.44
		QZ4P-DZ	QZ4P-TZ2P	QZ4P-QZ4P			
Ni	H	-338.26	-280.19	-261.85			
	C	1251.48	1601.31	1526.19			
V	H	415.44	377.61	374.87			
	C	-357.91	-434.70	-528.73			
Mn	H	-29.81	-18.01	-3.83			
	C	1371.26	1548.51	1398.72			

^a: $T = 298\text{K}$ for Ni and V. Shieldings and shifts for MnCp_2 were calculated at 390K . ^b: The first basis set listed corresponds to the metal or Silicon atom, and the second basis set listed was used for the Carbon and Hydrogen atoms.

3 Isotropic Hyperfine Couplings Constants of the Complexes

Table S12: STO Calculated HyFCCs for Metallocenes in (MHz)

		BP	PBE	B3LYP	PBE0	BHLYP
Ni	H	-4.3082	-4.0705	-3.6559	-3.6082	-3.0199
	C	3.5017	3.8968	5.0274	4.8514	5.7777
V	H	3.0452	3.0414	2.9306	2.8464	2.6590
	C	-0.7129	-0.6988	-0.6369	-1.0173	-0.7881
Mn	H	-0.0446	-0.0320	-0.0219	-0.0132	-0.0745
	C	1.2807	1.3617	1.5533	1.3916	1.6223

Table S13: GTO Calculated HyFCCs for Metallocenes in (MHz)

		BP	PBE	B3LYP	PBE0	BHLYP	CAM ^a	LC ^b	HF
Ni	H	-3.6217	-3.6487	-3.3776	-3.3450	-2.8645	-3.3144	-3.1367	-2.4814
	C	3.6283	4.0774	5.2130	5.0692	5.9545	5.3161	4.9608	4.7935
V	H	2.7521	2.7690	2.6808	2.6022	2.4511	2.6261	2.4746	2.2841
	C	-0.6793	-0.7897	-0.6360	-1.0550	-0.8150	-0.8350	-1.2876	-1.8983
Mn	H	-0.0130	-0.0104	-0.0448	-0.0366	-0.0939	-0.0640	-0.0606	-0.1183
	C	1.3204	1.3745	1.6042	1.4350	1.6746	1.5539	1.2939	1.1353

^a CAM-B3LYP ^b LC-PBE0

Table S14: STO Calculated Proton HyFCCs of Chromium Compounds in (MHz)

	Hydrogen #	BP	PBE	B3LYP	PBE0	BHLYP
CrL ¹	2	-1.6450	-1.4853	-1.0157	-1.1743	-1.1617
	4	-1.4423	-1.3447	-0.8310	-0.9180	-1.0007
	9,10	0.1062	0.1296	-0.0607	-0.1578	-0.1389
	5	-0.4167	-0.3867	-0.3207	-0.3987	-0.5757
	8,11	0.1061	0.1296	-0.0610	-0.1581	-0.1391
	6	0.0897	0.0660	0.1417	0.2100	0.4243
	3	0.6680	0.6097	-0.5427	0.6053	0.7940
	CrL ²	2	-1.6037	-1.4463	-1.0080	-1.1747
4		-1.3933	-1.2980	-0.8250	-0.9160	-1.0130
9,10		-0.0001	0.0253	-0.1964	-3.044	-0.3185
5		-0.4133	-0.3830	-0.3223	-0.4033	-0.5883
8,11		-0.002	0.0253	-0.1966	-0.3046	-0.3184
6		0.0890	0.0673	0.1430	0.2127	0.4353
3		0.6493	0.6060	0.5273	0.5903	0.7933

Table S15: STO Calculated FeL³ and FeL⁴ Amide and Amine Proton HyFCCs in (MHz) using PBE0 functional

Proton	H _t	H _c	H _a
HyFCC	0.3833	-0.0363	0.0373

Table S16: STO Calculated Planar and Saddled FeL⁵ Carbon HyFCCs in (MHz) using PBE0 functional

Carbon	α	β	<i>meso</i>
Planar High Spin	0.8442	1.0265	0.2915
Planar Low Spin	-1.0212	-0.3698	0.4341
Saddled High Spin	0.7080	1.0298	0.2787
Saddled Low Spin	-1.1135	-0.5395	0.4570

4 Metallocenes and Chromium Complexes with ZFS

Table S17: Calculated proton chemical shifts (ppm) of CrL¹ including ZFS effects

Functional	BP					PBE					
	H#	NoZ ^a	vW ^b	N ^c	P ^d	O ^e	NoZ	vW	N	P	O
2	-208.2	-208.4	-208.3	-208.3	-209.0	-187.1	-187.3	-187.2	-187.2	-187.9	
4	-182.9	-182.5	-182.5	-182.5	-182.5	-170.0	-169.6	-169.6	-169.7	-169.6	
9,10	-31.4	-31.0	-31.1	-31.1	-31.2	-26.5	-26.2	-26.2	-26.3	-26.4	
5	-47.6	-47.6	-47.5	-47.6	-47.5	-43.6	-43.6	-43.6	-43.6	-43.5	
8,11	62.8	62.8	62.8	62.8	62.8	64.1	64.2	64.1	64.2	64.1	
6	19.2	19.1	19.2	19.1	19.2	16.1	16.0	16.0	16.0	16.1	
3	95.4	95.5	95.5	95.5	95.4	87.7	87.8	87.8	87.8	87.7	

Functional	PBE0		B3LYP		BHLYP		LPV[1]			Exp.
	H#	NoZ	O	NoZ	O	NoZ	O	H* ^f	III* ^g	
2	-144.9	-146.0	-124.2	-125.6	-142.6	-144.5	-86.8	-103.7	-117.9	-78.0
4	-112.8	-112.4	-101.5	-101.2	-123.1	-122.8	-51.6	-67.9	-85.3	-56.0
9,10	-63.8	-63.7	-50.1	-50.0	-59.0	-59.0	-49.6	-53.9	-55.8	-41.1
5	-44.8	-44.6	-34.7	-34.5	-67.9	-67.7	-19.9	-25.9	-30.9	-15.8
8,11	25.3	25.3	37.2	37.3	25.7	25.9	34.4	25.7	26.8	27.6
6	35.2	35.3	26.1	26.2	63.2	63.3	19.7	21.4	24.2	15.3
3	87.2	87.2	78.9	78.8	111.7	111.6	57.2	62.2	66.9	51.8

^a: STO basis calculation without contribution from ZFS ^b: STO basis calculation including ZFS using method proscribed by Van Wüllen ^c: STO basis calculation including ZFS using method proscribed by Neese ^d: STO basis calculation including ZFS using method proscribed by Pederson ^e: STO basis shift calculation with ZFS obtained from ORCA calculation ^f: LPV's Gaussian 03[2] shift calculation with ZFS obtained from ORCA calculation, using an extrapolated approximation based upon the B3LYP and PBE functionals and The IGLO-III and IGLO-II basis sets for the ligand atoms and the basis set constructed by Munzarová and Kaupp[3] for Cr, and using an experimental X-ray structure for the heavy atoms with computationally optimized hydrogen positions.[1] ^g: As with "f", but using a fully optimized structure.[1] ^h: LPV's Gaussian 03 shift calculation with ZFS obtained from ORCA calculation, using the B3LYP functional with the IGLO-II basis set for the ligand atoms and the basis set constructed by Munzarová and Kaupp for Cr with a fully optimized structure.[1] All shifts were calculated at 298K.

Table S18: Calculated ZFS-including proton chemical shifts of CrL² in (ppm)^a

Functional H#	BP					PBE				
	NoZ	vW	N	P	O	NoZ	vW	N	P	O
2	-203.4	-203.7	-202.4	-203.6	-199.9	-182.5	-182.7	-181.5	-182.6	-178.9
4	-177.7	-177.6	-177.0	-177.7	-176.7	-165.0	-164.9	-164.3	-164.9	-164.0
9,10	-41.2	-41.4	-41.1	-41.3	-40.0	-36.4	-36.6	-36.3	-36.5	-35.3
5	-47.6	-47.4	-46.9	-47.5	-47.1	-43.6	-43.3	-42.9	-43.4	-43.1
8,11	44.8	44.5	43.3	44.6	42.9	46.8	46.5	45.3	46.6	44.9
6	19.2	19.4	19.7	19.3	19.4	16.3	16.5	16.8	16.4	16.5
3	93.8	93.9	94.5	93.9	95.1	88.1	88.1	88.8	88.1	89.4

Functional H#	PBE0		B3LYP		BHLYP		LPV[1]			Exp.
	NoZ	O	NoZ	O	NoZ	O	H*	III*	II	
2	-145.1	-144.0	-123.2	-121.5	-143.7	-142.4	-121.1	-118.8	-128.9	-74.0
4	-113.1	-112.4	-101.3	-100.5	-125.3	-124.7	-73.0	-70.5	-84.6	-58.1
9,10	-76.0	-75.2	-61.8	-60.9	-71.7	-71.1	-55.1	-66.3	-69.3	-48.9
5	-45.7	-45.4	-35.2	-34.8	-70.0	-69.6	-25.9	-27.5	-31.0	-17.2
8,11	-1.4	-2.3	13.0	11.8	-9.2	-10.2	10.6	4.7	5.7	11.2
6	35.8	35.9	26.4	26.6	65.1	65.3	22.6	21.8	24.0	15.5
3	85.9	86.5	77.5	78.3	112.4	113.1	62.4	60.5	65.4	51.3

^a: See footnotes for Table S17

Table S19: Calculated D Values for Chromium Compounds in (cm^{-1})

ORCA						
	BP		PBE			
	D^a	SS ^b	SO ^c	D	SS	SO
CrL ¹	1.19	0.46	0.72	1.21	0.46	0.74
CrL ²	4.39	-0.26	4.64	4.36	-0.26	4.62

ORCA									
	B3LYP			BHLYP			PBE0		
	D	SS	SO	D	SS	SO	D	SS	SO
CrL ¹	1.67	0.54	1.13	1.85	0.59	1.25	1.36	0.55	0.81
CrL ²	-2.91	-0.70	-2.84	-2.36	-0.14	-2.23	-2.38	-0.08	-2.30

ADF ^d						
	BP			PBE		
	vW	N	P	vW	N	P
CrL ¹	1.20	0.98	0.80	1.22	1.00	0.82
CrL ²	-1.47	4.39	-0.98	-1.46	4.34	-0.97

^a: Total D value. ^b: Spin-spin (SS) dipolar contribution to ZFS. ^c: Spin-orbit (SO) contribution to ZFS. ^d: Total calculated D value only includes the SO contribution.

Table S20: Calculated ZFS-including Chemical Shifts of Metallocenes in (ppm)^a

Functional	BP							
	No ZFS	vW	N	P	O	PV PBE0 ^b	HE B3LYP ^c	
Ni	H	-303.78	-303.85	-303.82	-303.85	-303.82	-242.62	-244.0
	C	1068.85	1031.06	1059.01	1050.05	1059.68	1401.24	1503.7
V	H	407.69	407.33	407.39	407.45	407.26	336.33	355.0
	C	-278.31	-280.08	-279.79	-279.49	-280.40	-429.17	-218.9
Mn	H	-7.93	-7.44	-7.41	-7.54	-8.75	5.18	-14.5
	C	1682.98	1688.78	1689.07	1687.62	1673.22	1820.40	2084.8

Functional	PBE							
	No ZFS	vW	N	P	O	PV PBE ^d	HE BP ^e	
Ni	H	-286.89	-286.98	-286.94	-286.97	-286.94	-258.24	-254.3
	C	1181.45	1143.37	1171.35	1162.51	1171.95	1276.26	1056.8
V	H	407.18	406.81	406.82	406.93	406.74	357.69	362.8
	C	-271.03	-272.96	-272.91	-272.31	-273.29	-287.57	-228.6
Mn	H	-4.06	-3.53	-3.50	-3.63	-4.69	12.12	-4.1
	C	1782.52	1788.76	1789.06	1787.51	1774.94	1728.18	1734.9

Functional	B3LYP		BHLYP		PBE0		
	No ZFS	O	No ZFS	O	No ZFS	O	
Ni	H	-260.59	-260.74	-221.40	-221.56	-258.32	-258.36
	C	1512.29	1492.59	1752.72	1745.42	1463.44	1460.70
V	H	391.77	391.13	355.08	354.58	380.60	380.01
	C	-233.05	-236.49	-311.74	-314.27	-434.56	-436.95
Mn	H	-1.01	1.18	-17.25	-13.64	1.70	3.61
	C	2023.06	2047.72	2108.06	2143.35	1822.57	1839.78

^a: See footnotes in Table S17; all shifts calculated at 298K ^b: PV's Gaussian 03 shift calculations with ZFS obtained from ORCA calculations, using the PBE0 functional with the IGLO-III basis set for the ligand atoms and the basis set constructed by Munzarová and Kaupp[3] for the metal center.[4] ^c: HE's Turbomole 5.6[5]/ReSpect[6] shift calculations using the B3LYP functional with the IGLO-III basis set for the ligand atoms and the basis set constructed by Munzarová and Kaupp[3] for the metal center.[7] ^d: As with "b" but for the PBE functional.[4] ^e: As with "c" but for the BP functional.[7]

5 Metallocene Chemical Shifts with an Alternative Reference Molecule

Table S21: STO calculated shieldings of paramagnetic metallocenes, TMS, and Ferrocene in (ppm).

		BP	PBE	B3LYP	PBE0	BHLYP
Ni	H	334.77	317.81	291.76	289.32	252.62
	C	-887.64	-999.74	-1331.26	-1277.49	-1566.97
V	H	-376.71	-376.26	-360.61	-349.61	-323.87
	C	459.52	452.74	414.08	620.51	497.49
Mn	H	35.65	32.63	30.58	28.34	43.05
	C	-1130.45	-1206.00	-1391.64	-1233.14	-1451.95
TMS	H	30.99	30.92	31.17	31.00	31.22
	C	181.21	181.71	181.03	185.96	185.75
Fe	H	27.39	27.34	27.80	27.70	28.24
	C	109.62	110.31	107.49	114.68	118.73

Table S22: STO calculated chemical shifts of paramagnetic metallocenes, TMS, and Ferrocene in (ppm).

Shifts with respect to TMS		BP	PBE	B3LYP	PBE0	BHLYP
FeCp ₂	H	3.60	3.58	3.37	3.30	2.98
	C	71.59	71.40	73.54	71.28	67.02
NiCp ₂	H	-303.78	-286.89	-260.59	-258.32	-221.40
	C	1068.85	1181.45	1512.29	1463.45	1752.72
VCp ₂	H	407.70	407.18	391.78	380.61	355.09
	C	-278.31	-271.03	-233.05	-434.55	-311.74
MnCp ₂	H	-4.66	-1.71	0.59	2.66	-11.83
	C	1311.66	1387.71	1572.67	1419.10	1637.70
$\delta\delta^a$	H	-0.40	-0.42	-0.63	-0.70	-1.02
	C	3.59	3.40	5.54	3.28	-0.98
Shifts with respect to FeCp ₂		BP	PBE	B3LYP	PBE0	BHLYP
Ni	H	-303.38	-286.47	-259.96	-257.62	-220.38
	C	1065.26	1178.05	1506.75	1460.17	1753.70
V	H	408.10	407.60	392.41	381.31	356.11
	C	-281.90	-274.43	-238.59	-437.83	-310.76
Mn	H	-4.26	-1.29	1.22	3.36	-10.81
	C	1308.07	1384.31	1567.13	1415.82	1638.68

^a: The difference between the experimentally measured chemical shifts of FeCp₂ and the calculated shifts, both with respect to TMS. The experimentally measured shifts are 4 ppm and 68 ppm, for proton and Carbon, respectively.[8]

6 FeL⁵ Carbon Chemical Shifts

Table S23: Planar and Saddled FeL⁵ Carbon Chemical Shifts (ppm) relative to the *meso* Carbon shifts^a

	Planar HS	Planar LS	Saddled HS	Saddled LS
Full, Finite Nuclei				
α	712.36	-681.03	564.14	-815.53
β	907.43	-400.99	930.14	-503.79
<i>meso</i>	0.00	0.00	0.00	0.00
Full, Point Nuclei				
α	712.56	-681.23	563.39	-815.90
β	907.53	-401.19	929.33	-504.12
<i>meso</i>	0.00	0.00	0.00	0.00
No ZFS				
α	699.37	-744.20	552.10	-803.89
β	902.66	-413.97	925.42	-513.49
<i>meso</i>	0.00	0.00	0.00	0.00
No Δg				
α	693.82	-732.73	547.15	-790.76
β	897.29	-407.21	919.72	-504.79
<i>meso</i>	0.00	0.00	0.00	0.00
No PSOSO				
α	691.60	-730.82	544.73	-788.85
β	899.30	-402.89	922.34	-500.29
<i>meso</i>	0.00	0.00	0.00	0.00
Nonrel.				
α	615.58	-720.38	464.84	-775.14
β	876.13	-400.56	897.41	-499.31
<i>meso</i>	0.00	0.00	0.00	0.00
CC ^b				
α	700.00			
β	820.00			
<i>meso</i>	0.00			
Exp ^c				
α	636.00			
β	776.00			
<i>meso</i>	0.00			

^a: Shifts were calculated with PBE0 at 303 K using STO basis functions. HS means $S = 5/2$, LS means $S = 3/2$. The ZFS tensor was calculated with ORCA. The shifts are presented as differences between the *meso* shift and the α and β shifts so that one could compare the ability of the methods to reproduce the differences among the shifts.

^b: Data from Chen & Chen,[9], calculated with ADF using TZP STO basis sets and the BP functional in the planar conformation with $S = 5/2$. ^c: Data from Mispelter et al.[10]

7 Solvent Effects on pNMR Shifts

Table S24: PBE0/STO calculated NMR shieldings for select complexes with solvent effects added using the conductor like screening model (COSMO)^a

		Diamagnetic	FC	PC	Total	
NiCp ₂	H	No Solvent	26.44	262.59	0.30	289.32
	C		95.25	-1403.81	31.06	-1277.49
	H	Toluene	26.26	261.15	0.30	287.70
	C		94.84	-1442.19	31.03	-1316.31
	H	Acetonitrile	26.11	259.83	0.30	286.23
	C		94.46	-1480.02	31.02	-1354.54
	H	Water	26.09	260.47	0.29	286.85
	C		94.38	-1476.53	30.90	-1351.25
FeL ³	H _c	No Solvent	24.97	7.15	-0.12	32.01
	H _t		25.08	-91.14	-0.57	-66.63
	H _c	Acetonitrile	25.13	8.16	-0.14	33.15
	H _t		25.15	-87.39	-0.67	-62.90
	H _c	Water	25.11	8.11	-0.13	33.09
	H _t		24.84	-87.36	-0.63	-63.16

^a: The three solvents chosen provide a wide range of dielectric constants while also being the set of solvents in which the experimental shifts of these two complexes were measured in their respective references. To provide a better direct comparison of these shieldings, geometries were not reoptimized for each solvent.

8 PNMRS_hift Results

The following data are the outputs of the pNMRS_hift program. The input data are echoed in the outputs as follows: Hyperfine tensors in units of MHz for each atom in the same order as in the *xyz* files, orbital shielding tensors in ppm for each atom in the same order as in the *xyz* files, *g*-shift tensors in ppt (parts per thousand), and where applicable the ZFS tensor in units of inverse cm. For each calculation, the first output line indicates the spin-state, molecule, STO or GTO basis, KS functional, and whether ZFS was excluded (No-ZFS) or included ('ORCA', or ADF with 'Neese', 'Pederson', or van Wüllen ('Van-Wullen') convention). Further details are provided in the main article. The outputs are in the following order:

```
3NiCp2-STO-BP-No-ZFS
3NiCp2-STO-BP-Neese
3NiCp2-STO-BP-ORCA
3NiCp2-STO-BP-Pederson
3NiCp2-STO-BP-Van-Wullen
3NiCp2-STO-PBE-No-ZFS
3NiCp2-STO-PBE-Neese
3NiCp2-STO-PBE-ORCA
3NiCp2-STO-PBE-Pederson
3NiCp2-STO-PBE-Van-Wullen
3NiCp2-STO-B3LYP-No-ZFS
3NiCp2-STO-B3LYP-ORCA
3NiCp2-STO-BHLYP-ORCA
3NiCp2-STO-BHLYP-No-ZFS
3NiCp2-STO-PBE0-No-ZFS
3NiCp2-STO-PBE0-ORCA
3NiCp2-STO-PBE0-No-G
3NiCp2-STO-PBE0-No-PSO
3NiCp2-STO-PBE0-No-ZORA
3NiCp2-GTO-B3LYP
3NiCp2-GTO-BHLYP
3NiCp2-GTO-BP
3NiCp2-GTO-CAM-B3LYP
3NiCp2-GTO-HF
3NiCp2-GTO-LC-PBE0
3NiCp2-GTO-PBE
3NiCp2-GTO-PBE0
4VCp2-STO-B3LYP-No-ZFS
4VCp2-STO-B3LYP-ORCA
4VCp2-STO-BHLYP-No-ZFS
4VCp2-STO-BHLYP-ORCA
4VCp2-STO-BP-No-ZFS
4VCp2-STO-BP-Neese
4VCp2-STO-BP-ORCA
```

4VCp2-STO-BP-Pederson
4VCp2-STO-BP-Van-Wullen
4VCp2-STO-PBE-No-ZFS
4VCp2-STO-PBE-Neese
4VCp2-STO-PBE-ORCA
4VCp2-STO-PBE-Pederson
4VCp2-STO-PBE-Van-Wullen
4VCp2-STO-PBE0-No-ZFS
4VCp2-STO-PBE0-ORCA
4VCp2-GTO-B3LYP
4VCp2-GTO-BHLYP
4VCp2-GTO-BP
4VCp2-GTO-CAM-B3LYP
4VCp2-GTO-HF
4VCp2-GTO-LC-PBE0
4VCp2-GTO-PBE
4VCp2-GTO-PBE0
6MnCp2-STO-B3LYP-No-ZFS
6MnCp2-STO-B3LYP-ORCA
6MnCp2-STO-BHLYP-No-ZFS
6MnCp2-STO-BHLYP-ORCA
6MnCp2-STO-BP-No-ZFS
6MnCp2-STO-BP-Neese
6MnCp2-STO-BP-ORCA
6MnCp2-STO-BP-Pederson
6MnCp2-STO-BP-Van-Wullen
6MnCp2-STO-PBE-No-ZFS
6MnCp2-STO-PBE-Neese
6MnCp2-STO-PBE-ORCA
6MnCp2-STO-PBE-Pederson
6MnCp2-STO-PBE-Van-Wullen
6MnCp2-STO-PBE0-No-ZFS
6MnCp2-STO-PBE0-ORCA
6MnCp2-GTO-BP
6MnCp2-GTO-PBE
6MnCp2-GTO-B3LYP
6MnCp2-GTO-BHLYP
6MnCp2-GTO-CAM-B3LYP
6MnCp2-GTO-HF
6MnCp2-GTO-LC-PBE0
6MnCp2-GTO-PBE0
CrL1-STO-B3LYP-No-ZFS
CrL1-STO-B3LYP-ORCA
CrL1-STO-BHLYP-No-ZFS

CrL1-STO-BHLYP-ORCA
CrL1-STO-BP-No-ZFS
CrL1-STO-BP-Neese
CrL1-STO-BP-ORCA
CrL1-STO-BP-Pederson
CrL1-STO-BP-Van-Wullen
CrL1-STO-PBE-No-ZFS
CrL1-STO-PBE-Neese
CrL1-STO-PBE-ORCA
CrL1-STO-PBE-Pederson
CrL1-STO-PBE-Van-Wullen
CrL1-STO-PBE0-No-ZFS
CrL1-STO-PBE0-ORCA
CrL2-STO-B3LYP-No-ZFS
CrL2-STO-B3LYP-ORCA
CrL2-STO-BHLYP-No-ZFS
CrL2-STO-BHLYP-ORCA
CrL2-STO-BP-No-ZFS
CrL2-STO-BP-Neese
CrL2-STO-BP-ORCA
CrL2-STO-BP-Pederson
CrL2-STO-BP-Van-Wullen
CrL2-STO-PBE-No-ZFS
CrL2-STO-PBE-Neese
CrL2-STO-PBE-ORCA
CrL2-STO-PBE-Pederson
CrL2-STO-PBE-Van-Wullen
CrL2-STO-PBE0-No-ZFS
CrL2-STO-PBE0-ORCA
FeL5-saddled-LS-STO-PBE0-Full-Finite
FeL5-saddled-LS-STO-PBE0-Full-ORCA
FeL5-saddled-LS-STO-PBE0-No-ZFS
FeL5-saddled-LS-STO-PBE0-No-G
FeL5-saddled-LS-STO-PBE0-No-PSOSO
FeL5-saddled-LS-STO-PBE0-No-ZORA
FeL5-saddled-HS-STO-PBE0-Full-Finite
FeL5-saddled-HS-STO-PBE0-Full-ORCA
FeL5-saddled-HS-STO-PBE0-No-ZFS
FeL5-saddled-HS-STO-PBE0-No-G
FeL5-saddled-HS-STO-PBE0-No-PSOSO
FeL5-saddled-HS-STO-PBE0-No-ZORA
FeL5-planar-LS-STO-PBE0-Full-Finite
FeL5-planar-LS-STO-PBE0-Full-ORCA
FeL5-planar-LS-STO-PBE0-No-ZFS

FeL5-planar-LS-STO-PBE0-No-G
FeL5-planar-LS-STO-PBE0-No-PSOSO
FeL5-planar-LS-STO-PBE0-No-ZORA
FeL5-planar-HS-STO-PBE0-Full-Finite
FeL5-planar-HS-STO-PBE0-Full-ORCA
FeL5-planar-HS-STO-PBE0-No-ZFS
FeL5-planar-HS-STO-PBE0-No-G
FeL5-planar-HS-STO-PBE0-No-PSOSO
FeL5-planar-HS-STO-PBE0-No-ZORA
FeL3-STO-PBE0-Full
FeL3-STO-PBE0-No-ZFS
FeL3-STO-PBE0-No-G
FeL3-STO-PBE0-No-PSOSO
FeL3-STO-PBE0-No-ZORA
FeL4-STO-PBE0-Full
FeL4-STO-PBE0-No-ZFS
FeL4-STO-PBE0-No-G
FeL4-STO-PBE0-No-PSOSO
FeL4-STO-PBE0-No-ZORA
3NiCp2-STO-PBE0-acetonitrile
3NiCp2-STO-PBE0-toluene
3NiCp2-STO-PBE0-water
FeL3-STO-PBE0-acetonitrile
FeL3-STO-PBE0-water
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3NiCp2-STO-PBE0-DZ-TZ2P
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6MnCp2-STO-PBE0-DZ-DZ
6MnCp2-STO-PBE0-DZ-TZ2P

6MnCp2-STO-PBE0-DZ-QZ4P
6MnCp2-STO-PBE0-TZ2P-DZ
6MnCp2-STO-PBE0-TZ2P-TZ2P
6MnCp2-STO-PBE0-TZ2P-QZ4P
6MnCp2-STO-PBE0-QZ4P-DZ
6MnCp2-STO-PBE0-QZ4P-TZ2P
6MnCp2-STO-PBE0-QZ4P-QZ4P

3NiCp2-STO-BP-No-ZFS
Temperature: 298
Spin: 1

atensor 1 Ni
91.408 0.000 0.011
0.000 91.409 0.005
0.011 0.005 4.605
-26.008 0.000 -0.003
0.000 -26.007 -0.001
-0.003 -0.001 -2.723

atensor 2 H
-7.577 -2.639 -0.909
-2.639 -1.093 2.557
-0.909 2.557 -4.183
-0.081 -0.031 -0.044
-0.031 -0.005 0.124
-0.010 0.029 0.010

atensor 3 C
-1.315 -0.231 -0.890
-0.231 -0.746 2.503
-0.890 2.503 12.941
-0.221 -0.032 -0.040
-0.032 -0.142 0.112
-0.014 0.040 -0.011

atensor 4 H
-0.161 0.229 -2.713
0.229 -8.509 -0.074
-2.713 -0.074 -4.183
0.006 0.003 -0.131
0.003 -0.091 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.663 0.020 -2.657
0.020 -1.396 -0.073
-2.657 -0.073 12.943
-0.131 0.003 -0.119
0.003 -0.232 -0.003
-0.043 -0.001 -0.011

atensor 6 H
-7.845 2.267 -0.768
2.267 -0.822 -2.603
-0.768 -2.603 -4.182
-0.084 0.027 -0.037
0.027 -0.002 -0.126
-0.009 -0.029 0.010

atensor 7 C
-1.337 0.199 -0.751
0.199 -0.720 -2.549

-0.751 -2.549 12.937
-0.224 0.028 -0.034
0.028 -0.139 -0.114
-0.012 -0.041 -0.011

atensor 8 H
-2.825 -3.898 2.239
-3.898 -5.840 -1.535
2.239 -1.535 -4.180
-0.025 -0.046 0.108
-0.046 -0.060 -0.074
0.025 -0.017 0.010

atensor 9 C
-0.896 -0.342 2.192
-0.342 -1.161 -1.502
2.192 -1.502 12.932
-0.163 -0.048 0.098
-0.048 -0.200 -0.067
0.035 -0.024 -0.011

atensor 10 H
-3.261 4.040 2.151
4.040 -5.405 1.655
2.151 1.655 -4.180
-0.030 0.047 0.104
0.047 -0.055 0.080
0.024 0.019 0.010

atensor 11 C
-0.936 0.355 2.106
0.355 -1.124 1.620
2.106 1.620 12.933
-0.168 0.049 0.094
0.049 -0.194 0.073
0.034 0.026 -0.011

atensor 12 H
-7.843 2.267 0.768
2.267 -0.823 2.604
0.768 2.604 -4.180
-0.084 0.027 0.037
0.027 -0.002 0.126
0.009 0.030 0.010

atensor 13 C
-1.336 0.199 0.752
0.199 -0.720 2.546
0.752 2.547 12.933
-0.224 0.028 0.034
0.028 -0.139 0.114
0.012 0.041 -0.011

atensor 14 H
-2.827 -3.899 -2.239
-3.899 -5.842 1.534
-2.239 1.534 -4.182
-0.025 -0.046 -0.108
-0.046 -0.060 0.074
-0.025 0.017 0.010

atensor 15 C
-0.898 -0.342 -2.190
-0.342 -1.162 1.500
-2.190 1.500 12.943
-0.163 -0.047 -0.098
-0.047 -0.200 0.067

-0.035 0.024 -0.011

atensor 16 H

-3.264 4.041 -2.150
4.041 -5.407 -1.655
-2.150 -1.655 -4.183
-0.030 0.047 -0.104
0.047 -0.055 -0.080
-0.024 -0.019 0.010

atensor 17 C

-0.937 0.354 -2.104
0.354 -1.124 -1.621
-2.104 -1.621 12.945
-0.168 0.049 -0.094
0.049 -0.194 -0.073
-0.034 -0.026 -0.011

atensor 18 H

-7.576 -2.639 0.909
-2.639 -1.093 -2.557
0.909 -2.557 -4.183
-0.081 -0.031 0.044
-0.031 -0.005 -0.124
0.010 -0.029 0.010

atensor 19 C

-1.313 -0.232 0.890
-0.232 -0.745 -2.503
0.890 -2.504 12.938
-0.221 -0.032 0.040
-0.032 -0.142 -0.112
0.014 -0.040 -0.011

atensor 20 C

-0.661 0.020 2.656
0.020 -1.394 0.072
2.656 0.072 12.929
-0.131 0.003 0.119
0.003 -0.232 0.003
0.042 0.001 -0.011

atensor 21 H

-0.159 0.229 2.713
0.229 -8.504 0.074
2.713 0.074 -4.179
0.006 0.003 0.131
0.003 -0.092 0.004
0.031 0.001 0.010

orbtensor 1 Ni

-7637.239 0.088 -0.143
0.088 -7637.215 -0.388
-0.143 -0.388 -640.027
2274.616 0.000 0.004
0.000 2274.616 0.001
0.004 0.001 2268.822

orbtensor 2 H

-0.660 3.615 0.721
3.615 -9.544 -2.028
0.721 -2.028 -0.579
26.378 -4.289 -1.194
-4.289 36.918 3.359
-1.194 3.359 25.650

orbtensor 3 C

-149.392	21.713	8.960
21.713	-202.728	-25.198
8.960	-25.198	-59.068
225.561	-5.606	-4.694
-5.606	239.336	13.203
-4.694	13.203	222.742

orbtensor 4 H

-10.821	-0.314	2.151
-0.314	0.616	0.059
2.151	0.059	-0.579
38.434	0.373	-3.563
0.373	24.864	-0.098
-3.563	-0.098	25.649

orbtensor 5 C

-210.401	-1.885	26.728
-1.885	-141.721	0.731
26.728	0.731	-59.065
241.318	0.487	-14.006
0.487	223.582	-0.384
-14.006	-0.384	222.742

orbtensor 6 H

-0.290	-3.107	0.608
-3.107	-9.912	2.064
0.608	2.064	-0.578
25.940	3.686	-1.008
3.686	37.356	-3.418
-1.008	-3.418	25.649

orbtensor 7 C

-147.154	-18.665	7.563
-18.665	-204.935	25.639
7.563	25.639	-59.065
224.988	4.818	-3.963
4.818	239.909	-13.439
-3.963	-13.439	222.742

orbtensor 8 H

-7.166	5.341	-1.775
5.341	-3.035	1.217
-1.775	1.217	-0.578
34.099	-6.338	2.940
-6.338	29.197	-2.015
2.940	-2.015	25.649

orbtensor 9 C

-188.432	32.080	-22.050
32.080	-163.626	15.112
-22.050	15.112	-59.067
235.649	-8.283	11.557
-8.283	229.243	-7.922
11.557	-7.922	222.743

orbtensor 10 H

-6.569	-5.535	-1.706
-5.535	-3.632	-1.312
-1.706	-1.312	-0.578
33.390	6.568	2.825
6.568	29.905	2.174
2.825	2.174	25.649

orbtensor 11 C

-184.851	-33.240	-21.191
-33.240	-167.226	-16.307
-21.191	-16.307	-59.067

234.723	8.584	11.105
8.584	230.169	8.545
11.105	8.545	222.743

orbtensor 12 H

-0.291	-3.107	-0.609
-3.107	-9.912	-2.065
-0.609	-2.065	-0.579
25.941	3.686	1.008
3.686	37.356	3.420
1.008	3.420	25.651

orbtensor 13 C

-147.137	-18.655	-7.557
-18.655	-204.923	-25.668
-7.557	-25.668	-59.070
224.987	4.818	3.961
4.818	239.906	13.442
3.961	13.442	222.746

orbtensor 14 H

-7.168	5.341	1.777
5.341	-3.036	-1.218
1.777	-1.218	-0.579
34.099	-6.337	-2.942
-6.337	29.197	2.016
-2.942	2.016	25.650

orbtensor 15 C

-188.470	32.072	22.084
32.072	-163.650	-15.136
22.084	-15.136	-59.074
235.652	-8.282	-11.560
-8.282	229.244	7.922
-11.560	7.922	222.744

orbtensor 16 H

-6.570	-5.536	1.707
-5.536	-3.634	1.313
1.707	1.313	-0.578
33.390	6.568	-2.826
6.568	29.907	-2.174
-2.826	-2.174	25.649

orbtensor 17 C

-184.889	-33.238	21.216
-33.238	-167.258	16.311
21.216	16.311	-59.065
234.724	8.585	-11.107
8.585	230.174	-8.544
-11.107	-8.544	222.741

orbtensor 18 H

-0.659	3.616	-0.721
3.616	-9.543	2.028
-0.721	2.028	-0.578
26.378	-4.289	1.193
-4.289	36.918	-3.358
1.193	-3.358	25.649

orbtensor 19 C

-149.372	21.706	-8.951
21.706	-202.727	25.199
-8.951	25.199	-59.063
225.558	-5.608	4.691
-5.608	239.336	-13.202
4.691	-13.202	222.740

```

orbtensor 20 C
-210.364  -1.881  -26.728
-1.881  -141.681  -0.738
-26.728  -0.738  -59.065
241.313   0.486  14.006
0.486   223.577   0.383
14.006   0.383  222.742

```

```

orbtensor 21 H
-10.818  -0.314  -2.151
-0.314   0.617  -0.059
-2.151  -0.059  -0.579
38.433   0.372   3.563
0.372   24.863   0.098
3.563   0.098  25.650

```

```

gtensor (ppt)
-0.045   0.000   0.000
0.000  -0.045   0.000
0.000   0.000  -0.207
40.993  -0.001   0.005
-0.001  40.993   0.003
0.005   0.003   1.027

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.2280	-3032.14233	35396.68058	223.32181	35620.00238	32587.86005
2	H	-4.3097	26.05433	308.75451	0.06438	308.81889	334.87322
3	C	3.5020	92.15033	-997.56492	17.69662	-979.86830	-887.71797
4	H	-4.3093	26.05433	308.73063	0.06470	308.79533	334.84966
5	C	3.5033	92.15167	-997.94473	17.69949	-980.24524	-888.09357
6	H	-4.3083	26.05500	308.65899	0.06470	308.72368	334.77868
7	C	3.5020	92.16167	-997.56492	17.69055	-979.87437	-887.71270
8	H	-4.3067	26.05533	308.53958	0.06427	308.60385	334.65918
9	C	3.5003	92.17000	-997.09016	17.68251	-979.40765	-887.23765
10	H	-4.3070	26.05500	308.56346	0.06439	308.62785	334.68285
11	C	3.5000	92.16367	-996.99521	17.68423	-979.31098	-887.14731
12	H	-4.3073	26.05533	308.58734	0.06461	308.65195	334.70728
13	C	3.5010	92.16967	-997.28006	17.68272	-979.59734	-887.42768
14	H	-4.3087	26.05433	308.68287	0.06459	308.74745	334.80179
15	C	3.5030	92.14867	-997.84978	17.69940	-980.15038	-888.00171
16	H	-4.3097	26.05467	308.75451	0.06500	308.81950	334.87417
17	C	3.5037	92.14233	-998.03968	17.70284	-980.33684	-888.19451
18	H	-4.3093	26.05500	308.73063	0.06437	308.79500	334.85000
19	C	3.5020	92.15733	-997.56492	17.69158	-979.87334	-887.71601
20	C	3.5000	92.17400	-996.99521	17.67687	-979.31834	-887.14434
21	H	-4.3060	26.05533	308.49182	0.06435	308.55617	334.61150
	ring 1H	-4.3082	26.05487	308.64943	0.06453	308.71397	334.76883
	ring 13C	3.5017	92.15893	-997.48896	17.69068	-979.79828	-887.63935

```

=====
3NiCp2-STO-BP-Neese
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
91.408 0.000 0.011
0.000 91.409 0.005
0.011 0.005 4.605

```

-26.008 0.000 -0.003
0.000 -26.007 -0.001
-0.003 -0.001 -2.723

atensor 2 H
-7.577 -2.639 -0.909
-2.639 -1.093 2.557
-0.909 2.557 -4.183
-0.081 -0.031 -0.044
-0.031 -0.005 0.124
-0.010 0.029 0.010

atensor 3 C
-1.315 -0.231 -0.890
-0.231 -0.746 2.503
-0.890 2.503 12.941
-0.221 -0.032 -0.040
-0.032 -0.142 0.112
-0.014 0.040 -0.011

atensor 4 H
-0.161 0.229 -2.713
0.229 -8.509 -0.074
-2.713 -0.074 -4.183
0.006 0.003 -0.131
0.003 -0.091 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.663 0.020 -2.657
0.020 -1.396 -0.073
-2.657 -0.073 12.943
-0.131 0.003 -0.119
0.003 -0.232 -0.003
-0.043 -0.001 -0.011

atensor 6 H
-7.845 2.267 -0.768
2.267 -0.822 -2.603
-0.768 -2.603 -4.182
-0.084 0.027 -0.037
0.027 -0.002 -0.126
-0.009 -0.029 0.010

atensor 7 C
-1.337 0.199 -0.751
0.199 -0.720 -2.549
-0.751 -2.549 12.937
-0.224 0.028 -0.034
0.028 -0.139 -0.114
-0.012 -0.041 -0.011

atensor 8 H
-2.825 -3.898 2.239
-3.898 -5.840 -1.535
2.239 -1.535 -4.180
-0.025 -0.046 0.108
-0.046 -0.060 -0.074
0.025 -0.017 0.010

atensor 9 C
-0.896 -0.342 2.192
-0.342 -1.161 -1.502
2.192 -1.502 12.932
-0.163 -0.048 0.098
-0.048 -0.200 -0.067
0.035 -0.024 -0.011

atensor 10 H
-3.261 4.040 2.151
4.040 -5.405 1.655
2.151 1.655 -4.180
-0.030 0.047 0.104
0.047 -0.055 0.080
0.024 0.019 0.010

atensor 11 C
-0.936 0.355 2.106
0.355 -1.124 1.620
2.106 1.620 12.933
-0.168 0.049 0.094
0.049 -0.194 0.073
0.034 0.026 -0.011

atensor 12 H
-7.843 2.267 0.768
2.267 -0.823 2.604
0.768 2.604 -4.180
-0.084 0.027 0.037
0.027 -0.002 0.126
0.009 0.030 0.010

atensor 13 C
-1.336 0.199 0.752
0.199 -0.720 2.546
0.752 2.547 12.933
-0.224 0.028 0.034
0.028 -0.139 0.114
0.012 0.041 -0.011

atensor 14 H
-2.827 -3.899 -2.239
-3.899 -5.842 1.534
-2.239 1.534 -4.182
-0.025 -0.046 -0.108
-0.046 -0.060 0.074
-0.025 0.017 0.010

atensor 15 C
-0.898 -0.342 -2.190
-0.342 -1.162 1.500
-2.190 1.500 12.943
-0.163 -0.047 -0.098
-0.047 -0.200 0.067
-0.035 0.024 -0.011

atensor 16 H
-3.264 4.041 -2.150
4.041 -5.407 -1.655
-2.150 -1.655 -4.183
-0.030 0.047 -0.104
0.047 -0.055 -0.080
-0.024 -0.019 0.010

atensor 17 C
-0.937 0.354 -2.104
0.354 -1.124 -1.621
-2.104 -1.621 12.945
-0.168 0.049 -0.094
0.049 -0.194 -0.073
-0.034 -0.026 -0.011

atensor 18 H
-7.576 -2.639 0.909

-2.639 -1.093 -2.557
0.909 -2.557 -4.183
-0.081 -0.031 0.044
-0.031 -0.005 -0.124
0.010 -0.029 0.010

atensor 19 C
-1.313 -0.232 0.890
-0.232 -0.745 -2.503
0.890 -2.504 12.938
-0.221 -0.032 0.040
-0.032 -0.142 -0.112
0.014 -0.040 -0.011

atensor 20 C
-0.661 0.020 2.656
0.020 -1.394 0.072
2.656 0.072 12.929
-0.131 0.003 0.119
0.003 -0.232 0.003
0.042 0.001 -0.011

atensor 21 H
-0.159 0.229 2.713
0.229 -8.504 0.074
2.713 0.074 -4.179
0.006 0.003 0.131
0.003 -0.092 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7637.239 0.088 -0.143
0.088 -7637.215 -0.388
-0.143 -0.388 -640.027
2274.616 0.000 0.004
0.000 2274.616 0.001
0.004 0.001 2268.822

orbtensor 2 H
-0.660 3.615 0.721
3.615 -9.544 -2.028
0.721 -2.028 -0.579
26.378 -4.289 -1.194
-4.289 36.918 3.359
-1.194 3.359 25.650

orbtensor 3 C
-149.392 21.713 8.960
21.713 -202.728 -25.198
8.960 -25.198 -59.068
225.561 -5.606 -4.694
-5.606 239.336 13.203
-4.694 13.203 222.742

orbtensor 4 H
-10.821 -0.314 2.151
-0.314 0.616 0.059
2.151 0.059 -0.579
38.434 0.373 -3.563
0.373 24.864 -0.098
-3.563 -0.098 25.649

orbtensor 5 C
-210.401 -1.885 26.728
-1.885 -141.721 0.731
26.728 0.731 -59.065
241.318 0.487 -14.006

0.487 223.582 -0.384
-14.006 -0.384 222.742

orbtensor 6 H
-0.290 -3.107 0.608
-3.107 -9.912 2.064
0.608 2.064 -0.578
25.940 3.686 -1.008
3.686 37.356 -3.418
-1.008 -3.418 25.649

orbtensor 7 C
-147.154 -18.665 7.563
-18.665 -204.935 25.639
7.563 25.639 -59.065
224.988 4.818 -3.963
4.818 239.909 -13.439
-3.963 -13.439 222.742

orbtensor 8 H
-7.166 5.341 -1.775
5.341 -3.035 1.217
-1.775 1.217 -0.578
34.099 -6.338 2.940
-6.338 29.197 -2.015
2.940 -2.015 25.649

orbtensor 9 C
-188.432 32.080 -22.050
32.080 -163.626 15.112
-22.050 15.112 -59.067
235.649 -8.283 11.557
-8.283 229.243 -7.922
11.557 -7.922 222.743

orbtensor 10 H
-6.569 -5.535 -1.706
-5.535 -3.632 -1.312
-1.706 -1.312 -0.578
33.390 6.568 2.825
6.568 29.905 2.174
2.825 2.174 25.649

orbtensor 11 C
-184.851 -33.240 -21.191
-33.240 -167.226 -16.307
-21.191 -16.307 -59.067
234.723 8.584 11.105
8.584 230.169 8.545
11.105 8.545 222.743

orbtensor 12 H
-0.291 -3.107 -0.609
-3.107 -9.912 -2.065
-0.609 -2.065 -0.579
25.941 3.686 1.008
3.686 37.356 3.420
1.008 3.420 25.651

orbtensor 13 C
-147.137 -18.655 -7.557
-18.655 -204.923 -25.668
-7.557 -25.668 -59.070
224.987 4.818 3.961
4.818 239.906 13.442
3.961 13.442 222.746

```

orbtensor 14 H
-7.168    5.341    1.777
5.341   -3.036   -1.218
1.777   -1.218   -0.579
34.099   -6.337   -2.942
-6.337   29.197    2.016
-2.942    2.016   25.650

orbtensor 15 C
-188.470   32.072   22.084
32.072  -163.650  -15.136
22.084  -15.136  -59.074
235.652   -8.282  -11.560
-8.282  229.244    7.922
-11.560    7.922  222.744

orbtensor 16 H
-6.570   -5.536    1.707
-5.536   -3.634    1.313
1.707    1.313   -0.578
33.390    6.568   -2.826
6.568   29.907   -2.174
-2.826   -2.174   25.649

orbtensor 17 C
-184.889  -33.238   21.216
-33.238  -167.258   16.311
21.216   16.311  -59.065
234.724    8.585  -11.107
8.585   230.174  -8.544
-11.107   -8.544  222.741

orbtensor 18 H
-0.659    3.616   -0.721
3.616   -9.543    2.028
-0.721    2.028   -0.578
26.378   -4.289    1.193
-4.289   36.918   -3.358
1.193   -3.358   25.649

orbtensor 19 C
-149.372   21.706   -8.951
21.706  -202.727   25.199
-8.951   25.199  -59.063
225.558   -5.608    4.691
-5.608   239.336  -13.202
4.691  -13.202  222.740

orbtensor 20 C
-210.364   -1.881   -26.728
-1.881  -141.681   -0.738
-26.728   -0.738  -59.065
241.313    0.486   14.006
0.486   223.577    0.383
14.006    0.383  222.742

orbtensor 21 H
-10.818   -0.314   -2.151
-0.314    0.617   -0.059
-2.151   -0.059   -0.579
38.433    0.372    3.563
0.372   24.863    0.098
3.563    0.098   25.650

gtensor (ppt)
-0.045    0.000    0.000
0.000   -0.045    0.000

```

```

0.000    0.000   -0.207
40.993   -0.001    0.005
-0.001   40.993    0.003
0.005    0.003    1.027

```

```

zfstensor (cm-1)
-1.531426    0.000043    0.002119
 0.000043   -1.531424    0.000094
 0.002119    0.000094    3.062850

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.2280	-3032.14233	35397.43401	347.77613	35745.21014	32713.06780
2	H	-4.3097	26.05433	308.76079	0.10012	308.86091	334.91524
3	C	3.5020	92.15033	-997.58871	27.55818	-970.03053	-877.88020
4	H	-4.3093	26.05433	308.73691	0.09989	308.83679	334.89113
5	C	3.5033	92.15167	-997.96853	27.55988	-970.40865	-878.25698
6	H	-4.3083	26.05500	308.66526	0.10036	308.76562	334.82062
7	C	3.5020	92.16167	-997.58871	27.54785	-970.04086	-877.87919
8	H	-4.3067	26.05533	308.54586	0.10075	308.64660	334.70193
9	C	3.5003	92.17000	-997.11394	27.53930	-969.57464	-877.40464
10	H	-4.3070	26.05500	308.56974	0.10101	308.67075	334.72575
11	C	3.5000	92.16367	-997.01898	27.54248	-969.47650	-877.31284
12	H	-4.3073	26.05533	308.59362	0.10097	308.69459	334.74992
13	C	3.5010	92.16967	-997.30385	27.53861	-969.76524	-877.59557
14	H	-4.3087	26.05433	308.68914	0.09998	308.78912	334.84345
15	C	3.5030	92.14867	-997.87357	27.56066	-970.31291	-878.16424
16	H	-4.3097	26.05467	308.76079	0.10041	308.86120	334.91587
17	C	3.5037	92.14233	-998.06348	27.56546	-970.49802	-878.35569
18	H	-4.3093	26.05500	308.73691	0.10043	308.83733	334.89233
19	C	3.5020	92.15733	-997.58871	27.55155	-970.03716	-877.87982
20	C	3.5000	92.17400	-997.01898	27.53141	-969.48758	-877.31358
21	H	-4.3060	26.05533	308.49809	0.10107	308.59917	334.65450
13C Average		3.5017	92.15893	-997.51275	27.54954	-969.96321	-877.80428
1H Average		-4.3082	26.05487	308.65571	0.10050	308.75621	334.81107

```

=====
3NiCp2-STO-BP-ORCA
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
91.408 0.000 0.011
0.000 91.409 0.005
0.011 0.005 4.605
-26.008 0.000 -0.003
0.000 -26.007 -0.001
-0.003 -0.001 -2.723

```

```

atensor 2 H
-7.577 -2.639 -0.909
-2.639 -1.093 2.557
-0.909 2.557 -4.183
-0.081 -0.031 -0.044
-0.031 -0.005 0.124
-0.010 0.029 0.010

```

```

atensor 3 C
-1.315 -0.231 -0.890
-0.231 -0.746 2.503

```

-0.890 2.503 12.941
-0.221 -0.032 -0.040
-0.032 -0.142 0.112
-0.014 0.040 -0.011

atensor 4 H
-0.161 0.229 -2.713
0.229 -8.509 -0.074
-2.713 -0.074 -4.183
0.006 0.003 -0.131
0.003 -0.091 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.663 0.020 -2.657
0.020 -1.396 -0.073
-2.657 -0.073 12.943
-0.131 0.003 -0.119
0.003 -0.232 -0.003
-0.043 -0.001 -0.011

atensor 6 H
-7.845 2.267 -0.768
2.267 -0.822 -2.603
-0.768 -2.603 -4.182
-0.084 0.027 -0.037
0.027 -0.002 -0.126
-0.009 -0.029 0.010

atensor 7 C
-1.337 0.199 -0.751
0.199 -0.720 -2.549
-0.751 -2.549 12.937
-0.224 0.028 -0.034
0.028 -0.139 -0.114
-0.012 -0.041 -0.011

atensor 8 H
-2.825 -3.898 2.239
-3.898 -5.840 -1.535
2.239 -1.535 -4.180
-0.025 -0.046 0.108
-0.046 -0.060 -0.074
0.025 -0.017 0.010

atensor 9 C
-0.896 -0.342 2.192
-0.342 -1.161 -1.502
2.192 -1.502 12.932
-0.163 -0.048 0.098
-0.048 -0.200 -0.067
0.035 -0.024 -0.011

atensor 10 H
-3.261 4.040 2.151
4.040 -5.405 1.655
2.151 1.655 -4.180
-0.030 0.047 0.104
0.047 -0.055 0.080
0.024 0.019 0.010

atensor 11 C
-0.936 0.355 2.106
0.355 -1.124 1.620
2.106 1.620 12.933
-0.168 0.049 0.094
0.049 -0.194 0.073

0.034 0.026 -0.011

atensor 12 H
-7.843 2.267 0.768
2.267 -0.823 2.604
0.768 2.604 -4.180
-0.084 0.027 0.037
0.027 -0.002 0.126
0.009 0.030 0.010

atensor 13 C
-1.336 0.199 0.752
0.199 -0.720 2.546
0.752 2.547 12.933
-0.224 0.028 0.034
0.028 -0.139 0.114
0.012 0.041 -0.011

atensor 14 H
-2.827 -3.899 -2.239
-3.899 -5.842 1.534
-2.239 1.534 -4.182
-0.025 -0.046 -0.108
-0.046 -0.060 0.074
-0.025 0.017 0.010

atensor 15 C
-0.898 -0.342 -2.190
-0.342 -1.162 1.500
-2.190 1.500 12.943
-0.163 -0.047 -0.098
-0.047 -0.200 0.067
-0.035 0.024 -0.011

atensor 16 H
-3.264 4.041 -2.150
4.041 -5.407 -1.655
-2.150 -1.655 -4.183
-0.030 0.047 -0.104
0.047 -0.055 -0.080
-0.024 -0.019 0.010

atensor 17 C
-0.937 0.354 -2.104
0.354 -1.124 -1.621
-2.104 -1.621 12.945
-0.168 0.049 -0.094
0.049 -0.194 -0.073
-0.034 -0.026 -0.011

atensor 18 H
-7.576 -2.639 0.909
-2.639 -1.093 -2.557
0.909 -2.557 -4.183
-0.081 -0.031 0.044
-0.031 -0.005 -0.124
0.010 -0.029 0.010

atensor 19 C
-1.313 -0.232 0.890
-0.232 -0.745 -2.503
0.890 -2.504 12.938
-0.221 -0.032 0.040
-0.032 -0.142 -0.112
0.014 -0.040 -0.011

atensor 20 C

-0.661 0.020 2.656
0.020 -1.394 0.072
2.656 0.072 12.929
-0.131 0.003 0.119
0.003 -0.232 0.003
0.042 0.001 -0.011

atensor 21 H
-0.159 0.229 2.713
0.229 -8.504 0.074
2.713 0.074 -4.179
0.006 0.003 0.131
0.003 -0.092 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7637.239 0.088 -0.143
0.088 -7637.215 -0.388
-0.143 -0.388 -640.027
2274.616 0.000 0.004
0.000 2274.616 0.001
0.004 0.001 2268.822

orbtensor 2 H
-0.660 3.615 0.721
3.615 -9.544 -2.028
0.721 -2.028 -0.579
26.378 -4.289 -1.194
-4.289 36.918 3.359
-1.194 3.359 25.650

orbtensor 3 C
-149.392 21.713 8.960
21.713 -202.728 -25.198
8.960 -25.198 -59.068
225.561 -5.606 -4.694
-5.606 239.336 13.203
-4.694 13.203 222.742

orbtensor 4 H
-10.821 -0.314 2.151
-0.314 0.616 0.059
2.151 0.059 -0.579
38.434 0.373 -3.563
0.373 24.864 -0.098
-3.563 -0.098 25.649

orbtensor 5 C
-210.401 -1.885 26.728
-1.885 -141.721 0.731
26.728 0.731 -59.065
241.318 0.487 -14.006
0.487 223.582 -0.384
-14.006 -0.384 222.742

orbtensor 6 H
-0.290 -3.107 0.608
-3.107 -9.912 2.064
0.608 2.064 -0.578
25.940 3.686 -1.008
3.686 37.356 -3.418
-1.008 -3.418 25.649

orbtensor 7 C
-147.154 -18.665 7.563
-18.665 -204.935 25.639
7.563 25.639 -59.065

224.988	4.818	-3.963
4.818	239.909	-13.439
-3.963	-13.439	222.742

orbtensor 8 H

-7.166	5.341	-1.775
5.341	-3.035	1.217
-1.775	1.217	-0.578
34.099	-6.338	2.940
-6.338	29.197	-2.015
2.940	-2.015	25.649

orbtensor 9 C

-188.432	32.080	-22.050
32.080	-163.626	15.112
-22.050	15.112	-59.067
235.649	-8.283	11.557
-8.283	229.243	-7.922
11.557	-7.922	222.743

orbtensor 10 H

-6.569	-5.535	-1.706
-5.535	-3.632	-1.312
-1.706	-1.312	-0.578
33.390	6.568	2.825
6.568	29.905	2.174
2.825	2.174	25.649

orbtensor 11 C

-184.851	-33.240	-21.191
-33.240	-167.226	-16.307
-21.191	-16.307	-59.067
234.723	8.584	11.105
8.584	230.169	8.545
11.105	8.545	222.743

orbtensor 12 H

-0.291	-3.107	-0.609
-3.107	-9.912	-2.065
-0.609	-2.065	-0.579
25.941	3.686	1.008
3.686	37.356	3.420
1.008	3.420	25.651

orbtensor 13 C

-147.137	-18.655	-7.557
-18.655	-204.923	-25.668
-7.557	-25.668	-59.070
224.987	4.818	3.961
4.818	239.906	13.442
3.961	13.442	222.746

orbtensor 14 H

-7.168	5.341	1.777
5.341	-3.036	-1.218
1.777	-1.218	-0.579
34.099	-6.337	-2.942
-6.337	29.197	2.016
-2.942	2.016	25.650

orbtensor 15 C

-188.470	32.072	22.084
32.072	-163.650	-15.136
22.084	-15.136	-59.074
235.652	-8.282	-11.560
-8.282	229.244	7.922
-11.560	7.922	222.744

orbtensor 16 H
-6.570 -5.536 1.707
-5.536 -3.634 1.313
1.707 1.313 -0.578
33.390 6.568 -2.826
6.568 29.907 -2.174
-2.826 -2.174 25.649

orbtensor 17 C
-184.889 -33.238 21.216
-33.238 -167.258 16.311
21.216 16.311 -59.065
234.724 8.585 -11.107
8.585 230.174 -8.544
-11.107 -8.544 222.741

orbtensor 18 H
-0.659 3.616 -0.721
3.616 -9.543 2.028
-0.721 2.028 -0.578
26.378 -4.289 1.193
-4.289 36.918 -3.358
1.193 -3.358 25.649

orbtensor 19 C
-149.372 21.706 -8.951
21.706 -202.727 25.199
-8.951 25.199 -59.063
225.558 -5.608 4.691
-5.608 239.336 -13.202
4.691 -13.202 222.740

orbtensor 20 C
-210.364 -1.881 -26.728
-1.881 -141.681 -0.738
-26.728 -0.738 -59.065
241.313 0.486 14.006
0.486 223.577 0.383
14.006 0.383 222.742

orbtensor 21 H
-10.818 -0.314 -2.151
-0.314 0.617 -0.059
-2.151 -0.059 -0.579
38.433 0.372 3.563
0.372 24.863 0.098
3.563 0.098 25.650

gtensor (ppt)
-0.045 0.000 0.000
0.000 -0.045 0.000
0.000 0.000 -0.207
40.993 -0.001 0.005
-0.001 40.993 0.003
0.005 0.003 1.027

zfstensor (cm-1)
44.250138 0.000339 0.001933
0.000339 44.249120 -0.000099
0.001933 -0.000099 48.533541

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.2280	-3032.14233	35397.44449	339.36972	35736.81421	32704.67188
2	H	-4.3097	26.05433	308.76088	0.09737	308.85825	334.91258
3	C	3.5020	92.15033	-997.58900	26.89176	-970.69725	-878.54691
4	H	-4.3093	26.05433	308.73700	0.09778	308.83478	334.88911
5	C	3.5033	92.15167	-997.96882	26.89401	-971.07481	-878.92315
6	H	-4.3083	26.05500	308.66535	0.09788	308.76323	334.81823
7	C	3.5020	92.16167	-997.58900	26.88222	-970.70679	-878.54512
8	H	-4.3067	26.05533	308.54595	0.09826	308.64420	334.69954
9	C	3.5003	92.17000	-997.11423	26.87358	-970.24065	-878.07065
10	H	-4.3070	26.05500	308.56983	0.09870	308.66853	334.72353
11	C	3.5000	92.16367	-997.01928	26.87649	-970.14279	-877.97912
12	H	-4.3073	26.05533	308.59371	0.09832	308.69203	334.74736
13	C	3.5010	92.16967	-997.30414	26.87260	-970.43155	-878.26188
14	H	-4.3087	26.05433	308.68923	0.09752	308.78675	334.84108
15	C	3.5030	92.14867	-997.87387	26.89447	-970.97940	-878.83073
16	H	-4.3097	26.05467	308.76088	0.09827	308.85915	334.91382
17	C	3.5037	92.14233	-998.06378	26.89954	-971.16423	-879.02190
18	H	-4.3093	26.05500	308.73700	0.09776	308.83476	334.88976
19	C	3.5020	92.15733	-997.58900	26.88564	-970.70336	-878.54603
20	C	3.5000	92.17400	-997.01928	26.86581	-970.15347	-877.97947
21	H	-4.3060	26.05533	308.49818	0.09883	308.59702	334.65235
13C Average		3.5017	92.15893	-997.51304	26.88361	-970.62943	-878.47050
1H Average		-4.3082	26.05487	308.65580	0.09807	308.75387	334.80874

=====
3NiCp2-STO-BP-Pederson
Temperature: 298
Spin: 1

atensor 1 Ni
91.408 0.000 0.011
0.000 91.409 0.005
0.011 0.005 4.605
-26.008 0.000 -0.003
0.000 -26.007 -0.001
-0.003 -0.001 -2.723

atensor 2 H
-7.577 -2.639 -0.909
-2.639 -1.093 2.557
-0.909 2.557 -4.183
-0.081 -0.031 -0.044
-0.031 -0.005 0.124
-0.010 0.029 0.010

atensor 3 C
-1.315 -0.231 -0.890
-0.231 -0.746 2.503
-0.890 2.503 12.941
-0.221 -0.032 -0.040
-0.032 -0.142 0.112
-0.014 0.040 -0.011

atensor 4 H
-0.161 0.229 -2.713
0.229 -8.509 -0.074
-2.713 -0.074 -4.183
0.006 0.003 -0.131
0.003 -0.091 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.663 0.020 -2.657

0.020 -1.396 -0.073
-2.657 -0.073 12.943
-0.131 0.003 -0.119
0.003 -0.232 -0.003
-0.043 -0.001 -0.011

atensor 6 H
-7.845 2.267 -0.768
2.267 -0.822 -2.603
-0.768 -2.603 -4.182
-0.084 0.027 -0.037
0.027 -0.002 -0.126
-0.009 -0.029 0.010

atensor 7 C
-1.337 0.199 -0.751
0.199 -0.720 -2.549
-0.751 -2.549 12.937
-0.224 0.028 -0.034
0.028 -0.139 -0.114
-0.012 -0.041 -0.011

atensor 8 H
-2.825 -3.898 2.239
-3.898 -5.840 -1.535
2.239 -1.535 -4.180
-0.025 -0.046 0.108
-0.046 -0.060 -0.074
0.025 -0.017 0.010

atensor 9 C
-0.896 -0.342 2.192
-0.342 -1.161 -1.502
2.192 -1.502 12.932
-0.163 -0.048 0.098
-0.048 -0.200 -0.067
0.035 -0.024 -0.011

atensor 10 H
-3.261 4.040 2.151
4.040 -5.405 1.655
2.151 1.655 -4.180
-0.030 0.047 0.104
0.047 -0.055 0.080
0.024 0.019 0.010

atensor 11 C
-0.936 0.355 2.106
0.355 -1.124 1.620
2.106 1.620 12.933
-0.168 0.049 0.094
0.049 -0.194 0.073
0.034 0.026 -0.011

atensor 12 H
-7.843 2.267 0.768
2.267 -0.823 2.604
0.768 2.604 -4.180
-0.084 0.027 0.037
0.027 -0.002 0.126
0.009 0.030 0.010

atensor 13 C
-1.336 0.199 0.752
0.199 -0.720 2.546
0.752 2.547 12.933
-0.224 0.028 0.034

0.028 -0.139 0.114
0.012 0.041 -0.011

atensor 14 H
-2.827 -3.899 -2.239
-3.899 -5.842 1.534
-2.239 1.534 -4.182
-0.025 -0.046 -0.108
-0.046 -0.060 0.074
-0.025 0.017 0.010

atensor 15 C
-0.898 -0.342 -2.190
-0.342 -1.162 1.500
-2.190 1.500 12.943
-0.163 -0.047 -0.098
-0.047 -0.200 0.067
-0.035 0.024 -0.011

atensor 16 H
-3.264 4.041 -2.150
4.041 -5.407 -1.655
-2.150 -1.655 -4.183
-0.030 0.047 -0.104
0.047 -0.055 -0.080
-0.024 -0.019 0.010

atensor 17 C
-0.937 0.354 -2.104
0.354 -1.124 -1.621
-2.104 -1.621 12.945
-0.168 0.049 -0.094
0.049 -0.194 -0.073
-0.034 -0.026 -0.011

atensor 18 H
-7.576 -2.639 0.909
-2.639 -1.093 -2.557
0.909 -2.557 -4.183
-0.081 -0.031 0.044
-0.031 -0.005 -0.124
0.010 -0.029 0.010

atensor 19 C
-1.313 -0.232 0.890
-0.232 -0.745 -2.503
0.890 -2.504 12.938
-0.221 -0.032 0.040
-0.032 -0.142 -0.112
0.014 -0.040 -0.011

atensor 20 C
-0.661 0.020 2.656
0.020 -1.394 0.072
2.656 0.072 12.929
-0.131 0.003 0.119
0.003 -0.232 0.003
0.042 0.001 -0.011

atensor 21 H
-0.159 0.229 2.713
0.229 -8.504 0.074
2.713 0.074 -4.179
0.006 0.003 0.131
0.003 -0.092 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7637.239 0.088 -0.143
0.088 -7637.215 -0.388
-0.143 -0.388 -640.027
2274.616 0.000 0.004
0.000 2274.616 0.001
0.004 0.001 2268.822

orbtensor 2 H
-0.660 3.615 0.721
3.615 -9.544 -2.028
0.721 -2.028 -0.579
26.378 -4.289 -1.194
-4.289 36.918 3.359
-1.194 3.359 25.650

orbtensor 3 C
-149.392 21.713 8.960
21.713 -202.728 -25.198
8.960 -25.198 -59.068
225.561 -5.606 -4.694
-5.606 239.336 13.203
-4.694 13.203 222.742

orbtensor 4 H
-10.821 -0.314 2.151
-0.314 0.616 0.059
2.151 0.059 -0.579
38.434 0.373 -3.563
0.373 24.864 -0.098
-3.563 -0.098 25.649

orbtensor 5 C
-210.401 -1.885 26.728
-1.885 -141.721 0.731
26.728 0.731 -59.065
241.318 0.487 -14.006
0.487 223.582 -0.384
-14.006 -0.384 222.742

orbtensor 6 H
-0.290 -3.107 0.608
-3.107 -9.912 2.064
0.608 2.064 -0.578
25.940 3.686 -1.008
3.686 37.356 -3.418
-1.008 -3.418 25.649

orbtensor 7 C
-147.154 -18.665 7.563
-18.665 -204.935 25.639
7.563 25.639 -59.065
224.988 4.818 -3.963
4.818 239.909 -13.439
-3.963 -13.439 222.742

orbtensor 8 H
-7.166 5.341 -1.775
5.341 -3.035 1.217
-1.775 1.217 -0.578
34.099 -6.338 2.940
-6.338 29.197 -2.015
2.940 -2.015 25.649

orbtensor 9 C
-188.432 32.080 -22.050
32.080 -163.626 15.112

-22.050	15.112	-59.067
235.649	-8.283	11.557
-8.283	229.243	-7.922
11.557	-7.922	222.743

orbtensor 10 H

-6.569	-5.535	-1.706
-5.535	-3.632	-1.312
-1.706	-1.312	-0.578
33.390	6.568	2.825
6.568	29.905	2.174
2.825	2.174	25.649

orbtensor 11 C

-184.851	-33.240	-21.191
-33.240	-167.226	-16.307
-21.191	-16.307	-59.067
234.723	8.584	11.105
8.584	230.169	8.545
11.105	8.545	222.743

orbtensor 12 H

-0.291	-3.107	-0.609
-3.107	-9.912	-2.065
-0.609	-2.065	-0.579
25.941	3.686	1.008
3.686	37.356	3.420
1.008	3.420	25.651

orbtensor 13 C

-147.137	-18.655	-7.557
-18.655	-204.923	-25.668
-7.557	-25.668	-59.070
224.987	4.818	3.961
4.818	239.906	13.442
3.961	13.442	222.746

orbtensor 14 H

-7.168	5.341	1.777
5.341	-3.036	-1.218
1.777	-1.218	-0.579
34.099	-6.337	-2.942
-6.337	29.197	2.016
-2.942	2.016	25.650

orbtensor 15 C

-188.470	32.072	22.084
32.072	-163.650	-15.136
22.084	-15.136	-59.074
235.652	-8.282	-11.560
-8.282	229.244	7.922
-11.560	7.922	222.744

orbtensor 16 H

-6.570	-5.536	1.707
-5.536	-3.634	1.313
1.707	1.313	-0.578
33.390	6.568	-2.826
6.568	29.907	-2.174
-2.826	-2.174	25.649

orbtensor 17 C

-184.889	-33.238	21.216
-33.238	-167.258	16.311
21.216	16.311	-59.065
234.724	8.585	-11.107
8.585	230.174	-8.544

-11.107 -8.544 222.741

orbtensor 18 H

-0.659 3.616 -0.721
3.616 -9.543 2.028
-0.721 2.028 -0.578
26.378 -4.289 1.193
-4.289 36.918 -3.358
1.193 -3.358 25.649

orbtensor 19 C

-149.372 21.706 -8.951
21.706 -202.727 25.199
-8.951 25.199 -59.063
225.558 -5.608 4.691
-5.608 239.336 -13.202
4.691 -13.202 222.740

orbtensor 20 C

-210.364 -1.881 -26.728
-1.881 -141.681 -0.738
-26.728 -0.738 -59.065
241.313 0.486 14.006
0.486 223.577 0.383
14.006 0.383 222.742

orbtensor 21 H

-10.818 -0.314 -2.151
-0.314 0.617 -0.059
-2.151 -0.059 -0.579
38.433 0.372 3.563
0.372 24.863 0.098
3.563 0.098 25.650

gtensor (ppt)

-0.045 0.000 0.000
0.000 -0.045 0.000
0.000 0.000 -0.207
40.993 -0.001 0.005
-0.001 40.993 0.003
0.005 0.003 1.027

zfstensor (cm-1)

-2.919920 -0.000060 0.000535
-0.000060 -2.919899 0.000434
0.000535 0.000434 5.839818

averaging

13C Average:3,5,7,9,11,13,15,17,19,20

1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.2280	-3032.14233	35396.42656	460.57765	35857.00420	32824.86187
2	H	-4.3097	26.05433	308.75200	0.13302	308.88502	334.93935
3	C	3.5020	92.15033	-997.56032	36.49813	-961.06218	-868.91185
4	H	-4.3093	26.05433	308.72812	0.13289	308.86101	334.91535
5	C	3.5033	92.15167	-997.94012	36.50135	-961.43877	-869.28711
6	H	-4.3083	26.05500	308.65648	0.13288	308.78936	334.84436
7	C	3.5020	92.16167	-997.56032	36.48307	-961.07724	-868.91558
8	H	-4.3067	26.05533	308.53707	0.13290	308.66997	334.72531
9	C	3.5003	92.17000	-997.08556	36.46937	-960.61619	-868.44619
10	H	-4.3070	26.05500	308.56095	0.13330	308.69425	334.74925
11	C	3.5000	92.16367	-996.99061	36.47434	-960.51627	-868.35260
12	H	-4.3073	26.05533	308.58484	0.13366	308.71849	334.77382

13	C	3.5010	92.16967	-997.27546	36.47069	-960.80477	-868.63511
14	H	-4.3087	26.05433	308.68036	0.13309	308.81345	334.86778
15	C	3.5030	92.14867	-997.84517	36.50238	-961.34280	-869.19413
16	H	-4.3097	26.05467	308.75200	0.13329	308.88529	334.93995
17	C	3.5037	92.14233	-998.03507	36.50783	-961.52724	-869.38491
18	H	-4.3093	26.05500	308.72812	0.13270	308.86082	334.91582
19	C	3.5020	92.15733	-997.56032	36.48653	-961.07378	-868.91645
20	C	3.5000	92.17400	-996.99061	36.45883	-960.53178	-868.35778
21	H	-4.3060	26.05533	308.48931	0.13323	308.62254	334.67788
13C Average		3.5017	92.15893	-997.48436	36.48525	-960.99910	-868.84017
1H Average		-4.3082	26.05487	308.64692	0.13310	308.78002	334.83489

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3NiCp2-STO-BP-Van-Wullen

Temperature: 298

Spin: 1

atensor 1 Ni

91.408 0.000 0.011
0.000 91.409 0.005
0.011 0.005 4.605
-26.008 0.000 -0.003
0.000 -26.007 -0.001
-0.003 -0.001 -2.723

atensor 2 H

-7.577 -2.639 -0.909
-2.639 -1.093 2.557
-0.909 2.557 -4.183
-0.081 -0.031 -0.044
-0.031 -0.005 0.124
-0.010 0.029 0.010

atensor 3 C

-1.315 -0.231 -0.890
-0.231 -0.746 2.503
-0.890 2.503 12.941
-0.221 -0.032 -0.040
-0.032 -0.142 0.112
-0.014 0.040 -0.011

atensor 4 H

-0.161 0.229 -2.713
0.229 -8.509 -0.074
-2.713 -0.074 -4.183
0.006 0.003 -0.131
0.003 -0.091 -0.004
-0.031 -0.001 0.010

atensor 5 C

-0.663 0.020 -2.657
0.020 -1.396 -0.073
-2.657 -0.073 12.943
-0.131 0.003 -0.119
0.003 -0.232 -0.003
-0.043 -0.001 -0.011

atensor 6 H

-7.845 2.267 -0.768
2.267 -0.822 -2.603
-0.768 -2.603 -4.182
-0.084 0.027 -0.037
0.027 -0.002 -0.126
-0.009 -0.029 0.010

atensor 7 C

-1.337 0.199 -0.751
0.199 -0.720 -2.549
-0.751 -2.549 12.937
-0.224 0.028 -0.034
0.028 -0.139 -0.114
-0.012 -0.041 -0.011

atensor 8 H
-2.825 -3.898 2.239
-3.898 -5.840 -1.535
2.239 -1.535 -4.180
-0.025 -0.046 0.108
-0.046 -0.060 -0.074
0.025 -0.017 0.010

atensor 9 C
-0.896 -0.342 2.192
-0.342 -1.161 -1.502
2.192 -1.502 12.932
-0.163 -0.048 0.098
-0.048 -0.200 -0.067
0.035 -0.024 -0.011

atensor 10 H
-3.261 4.040 2.151
4.040 -5.405 1.655
2.151 1.655 -4.180
-0.030 0.047 0.104
0.047 -0.055 0.080
0.024 0.019 0.010

atensor 11 C
-0.936 0.355 2.106
0.355 -1.124 1.620
2.106 1.620 12.933
-0.168 0.049 0.094
0.049 -0.194 0.073
0.034 0.026 -0.011

atensor 12 H
-7.843 2.267 0.768
2.267 -0.823 2.604
0.768 2.604 -4.180
-0.084 0.027 0.037
0.027 -0.002 0.126
0.009 0.030 0.010

atensor 13 C
-1.336 0.199 0.752
0.199 -0.720 2.546
0.752 2.547 12.933
-0.224 0.028 0.034
0.028 -0.139 0.114
0.012 0.041 -0.011

atensor 14 H
-2.827 -3.899 -2.239
-3.899 -5.842 1.534
-2.239 1.534 -4.182
-0.025 -0.046 -0.108
-0.046 -0.060 0.074
-0.025 0.017 0.010

atensor 15 C
-0.898 -0.342 -2.190
-0.342 -1.162 1.500
-2.190 1.500 12.943

-0.163 -0.047 -0.098
-0.047 -0.200 0.067
-0.035 0.024 -0.011

atensor 16 H
-3.264 4.041 -2.150
4.041 -5.407 -1.655
-2.150 -1.655 -4.183
-0.030 0.047 -0.104
0.047 -0.055 -0.080
-0.024 -0.019 0.010

atensor 17 C
-0.937 0.354 -2.104
0.354 -1.124 -1.621
-2.104 -1.621 12.945
-0.168 0.049 -0.094
0.049 -0.194 -0.073
-0.034 -0.026 -0.011

atensor 18 H
-7.576 -2.639 0.909
-2.639 -1.093 -2.557
0.909 -2.557 -4.183
-0.081 -0.031 0.044
-0.031 -0.005 -0.124
0.010 -0.029 0.010

atensor 19 C
-1.313 -0.232 0.890
-0.232 -0.745 -2.503
0.890 -2.504 12.938
-0.221 -0.032 0.040
-0.032 -0.142 -0.112
0.014 -0.040 -0.011

atensor 20 C
-0.661 0.020 2.656
0.020 -1.394 0.072
2.656 0.072 12.929
-0.131 0.003 0.119
0.003 -0.232 0.003
0.042 0.001 -0.011

atensor 21 H
-0.159 0.229 2.713
0.229 -8.504 0.074
2.713 0.074 -4.179
0.006 0.003 0.131
0.003 -0.092 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7637.239 0.088 -0.143
0.088 -7637.215 -0.388
-0.143 -0.388 -640.027
2274.616 0.000 0.004
0.000 2274.616 0.001
0.004 0.001 2268.822

orbtensor 2 H
-0.660 3.615 0.721
3.615 -9.544 -2.028
0.721 -2.028 -0.579
26.378 -4.289 -1.194
-4.289 36.918 3.359
-1.194 3.359 25.650

orbtensor 3 C
-149.392 21.713 8.960
21.713 -202.728 -25.198
8.960 -25.198 -59.068
225.561 -5.606 -4.694
-5.606 239.336 13.203
-4.694 13.203 222.742

orbtensor 4 H
-10.821 -0.314 2.151
-0.314 0.616 0.059
2.151 0.059 -0.579
38.434 0.373 -3.563
0.373 24.864 -0.098
-3.563 -0.098 25.649

orbtensor 5 C
-210.401 -1.885 26.728
-1.885 -141.721 0.731
26.728 0.731 -59.065
241.318 0.487 -14.006
0.487 223.582 -0.384
-14.006 -0.384 222.742

orbtensor 6 H
-0.290 -3.107 0.608
-3.107 -9.912 2.064
0.608 2.064 -0.578
25.940 3.686 -1.008
3.686 37.356 -3.418
-1.008 -3.418 25.649

orbtensor 7 C
-147.154 -18.665 7.563
-18.665 -204.935 25.639
7.563 25.639 -59.065
224.988 4.818 -3.963
4.818 239.909 -13.439
-3.963 -13.439 222.742

orbtensor 8 H
-7.166 5.341 -1.775
5.341 -3.035 1.217
-1.775 1.217 -0.578
34.099 -6.338 2.940
-6.338 29.197 -2.015
2.940 -2.015 25.649

orbtensor 9 C
-188.432 32.080 -22.050
32.080 -163.626 15.112
-22.050 15.112 -59.067
235.649 -8.283 11.557
-8.283 229.243 -7.922
11.557 -7.922 222.743

orbtensor 10 H
-6.569 -5.535 -1.706
-5.535 -3.632 -1.312
-1.706 -1.312 -0.578
33.390 6.568 2.825
6.568 29.905 2.174
2.825 2.174 25.649

orbtensor 11 C
-184.851 -33.240 -21.191

-33.240	-167.226	-16.307
-21.191	-16.307	-59.067
234.723	8.584	11.105
8.584	230.169	8.545
11.105	8.545	222.743

orbtensor 12 H

-0.291	-3.107	-0.609
-3.107	-9.912	-2.065
-0.609	-2.065	-0.579
25.941	3.686	1.008
3.686	37.356	3.420
1.008	3.420	25.651

orbtensor 13 C

-147.137	-18.655	-7.557
-18.655	-204.923	-25.668
-7.557	-25.668	-59.070
224.987	4.818	3.961
4.818	239.906	13.442
3.961	13.442	222.746

orbtensor 14 H

-7.168	5.341	1.777
5.341	-3.036	-1.218
1.777	-1.218	-0.579
34.099	-6.337	-2.942
-6.337	29.197	2.016
-2.942	2.016	25.650

orbtensor 15 C

-188.470	32.072	22.084
32.072	-163.650	-15.136
22.084	-15.136	-59.074
235.652	-8.282	-11.560
-8.282	229.244	7.922
-11.560	7.922	222.744

orbtensor 16 H

-6.570	-5.536	1.707
-5.536	-3.634	1.313
1.707	1.313	-0.578
33.390	6.568	-2.826
6.568	29.907	-2.174
-2.826	-2.174	25.649

orbtensor 17 C

-184.889	-33.238	21.216
-33.238	-167.258	16.311
21.216	16.311	-59.065
234.724	8.585	-11.107
8.585	230.174	-8.544
-11.107	-8.544	222.741

orbtensor 18 H

-0.659	3.616	-0.721
3.616	-9.543	2.028
-0.721	2.028	-0.578
26.378	-4.289	1.193
-4.289	36.918	-3.358
1.193	-3.358	25.649

orbtensor 19 C

-149.372	21.706	-8.951
21.706	-202.727	25.199
-8.951	25.199	-59.063
225.558	-5.608	4.691

-5.608 239.336 -13.202
 4.691 -13.202 222.740

orbtensor 20 C
 -210.364 -1.881 -26.728
 -1.881 -141.681 -0.738
 -26.728 -0.738 -59.065
 241.313 0.486 14.006
 0.486 223.577 0.383
 14.006 0.383 222.742

orbtensor 21 H
 -10.818 -0.314 -2.151
 -0.314 0.617 -0.059
 -2.151 -0.059 -0.579
 38.433 0.372 3.563
 0.372 24.863 0.098
 3.563 0.098 25.650

gtensor (ppt)
 -0.045 0.000 0.000
 0.000 -0.045 0.000
 0.000 0.000 -0.207
 40.993 -0.001 0.005
 -0.001 40.993 0.003
 0.005 0.003 1.027

zfstensor (cm-1)
 -5.839831 -0.000116 0.001071
 -0.000116 -5.839786 0.000870
 0.001071 0.000870 11.679617

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.2280	-3032.14233	35388.99253	697.57253	36086.56506	33054.42272
2	H	-4.3097	26.05433	308.68715	0.20159	308.88874	334.94307
3	C	3.5020	92.15033	-997.35081	55.27893	-942.07188	-849.92154
4	H	-4.3093	26.05433	308.66328	0.20101	308.86429	334.91862
5	C	3.5033	92.15167	-997.73053	55.28248	-942.44805	-850.29639
6	H	-4.3083	26.05500	308.59165	0.20099	308.79264	334.84764
7	C	3.5020	92.16167	-997.35081	55.25488	-942.09593	-849.93426
8	H	-4.3067	26.05533	308.47227	0.20145	308.67373	334.72906
9	C	3.5003	92.17000	-996.87615	55.23551	-941.64064	-849.47064
10	H	-4.3070	26.05500	308.49615	0.20213	308.69828	334.75328
11	C	3.5000	92.16367	-996.78122	55.24374	-941.53748	-849.37381
12	H	-4.3073	26.05533	308.52003	0.20263	308.72266	334.77799
13	C	3.5010	92.16967	-997.06601	55.23795	-941.82806	-849.65839
14	H	-4.3087	26.05433	308.61553	0.20152	308.81705	334.87138
15	C	3.5030	92.14867	-997.63560	55.28463	-942.35098	-850.20231
16	H	-4.3097	26.05467	308.68715	0.20151	308.88866	334.94333
17	C	3.5037	92.14233	-997.82546	55.29210	-942.53337	-850.39103
18	H	-4.3093	26.05500	308.66328	0.20095	308.86423	334.91923
19	C	3.5020	92.15733	-997.35081	55.26077	-942.09003	-849.93270
20	C	3.5000	92.17400	-996.78122	55.22009	-941.56112	-849.38712
21	H	-4.3060	26.05533	308.42452	0.20203	308.62656	334.68189
13C Average		3.5017	92.15893	-997.27486	55.25911	-942.01575	-849.85682
1H Average		-4.3082	26.05487	308.58210	0.20158	308.78368	334.83855

3NiCp2-STO-PBE-No-ZFS

Temperature: 298
Spin: 1

atensor 1 Ni
91.492 0.000 0.011
0.000 91.492 0.006
0.011 0.006 4.436
-26.459 0.000 -0.003
0.000 -26.459 -0.002
-0.003 -0.002 -2.693

atensor 2 H
-7.318 -2.614 -0.914
-2.614 -0.894 2.571
-0.914 2.571 -3.927
-0.082 -0.032 -0.045
-0.032 -0.004 0.126
-0.010 0.029 0.010

atensor 3 C
-0.832 -0.227 -0.894
-0.227 -0.275 2.514
-0.894 2.514 13.176
-0.223 -0.033 -0.041
-0.033 -0.142 0.114
-0.014 0.040 -0.011

atensor 4 H
0.030 0.227 -2.728
0.227 -8.242 -0.075
-2.728 -0.075 -3.927
0.007 0.003 -0.134
0.003 -0.093 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.195 0.020 -2.667
0.020 -0.912 -0.073
-2.667 -0.073 13.176
-0.130 0.003 -0.121
0.003 -0.235 -0.003
-0.042 -0.001 -0.011

atensor 6 H
-7.584 2.247 -0.772
2.247 -0.626 -2.617
-0.772 -2.618 -3.926
-0.085 0.027 -0.038
0.027 -0.001 -0.128
-0.009 -0.030 0.010

atensor 7 C
-0.854 0.195 -0.754
0.195 -0.250 -2.559
-0.754 -2.560 13.172
-0.226 0.028 -0.034
0.028 -0.139 -0.116
-0.012 -0.041 -0.011

atensor 8 H
-2.610 -3.862 2.251
-3.862 -5.597 -1.543
2.251 -1.543 -3.925
-0.025 -0.047 0.110
-0.047 -0.061 -0.076
0.025 -0.017 0.010

atensor 9 C
-0.423 -0.335 2.201
-0.335 -0.682 -1.509
2.201 -1.509 13.166
-0.164 -0.049 0.100
-0.049 -0.201 -0.069
0.035 -0.024 -0.011

atensor 10 H
-3.042 4.003 2.163
4.003 -5.166 1.664
2.163 1.664 -3.925
-0.030 0.049 0.106
0.049 -0.056 0.082
0.024 0.019 0.010

atensor 11 C
-0.462 0.347 2.115
0.347 -0.646 1.626
2.115 1.626 13.168
-0.169 0.051 0.096
0.051 -0.196 0.074
0.034 0.026 -0.011

atensor 12 H
-7.581 2.247 0.772
2.247 -0.626 2.618
0.772 2.618 -3.924
-0.085 0.027 0.038
0.027 -0.001 0.128
0.009 0.030 0.010

atensor 13 C
-0.853 0.195 0.755
0.195 -0.251 2.557
0.755 2.557 13.167
-0.226 0.028 0.034
0.028 -0.138 0.116
0.012 0.041 -0.011

atensor 14 H
-2.613 -3.863 -2.251
-3.863 -5.600 1.543
-2.251 1.543 -3.927
-0.025 -0.047 -0.110
-0.047 -0.061 0.076
-0.025 0.017 0.010

atensor 15 C
-0.424 -0.335 -2.199
-0.335 -0.683 1.506
-2.199 1.507 13.177
-0.164 -0.049 -0.100
-0.049 -0.201 0.069
-0.035 0.024 -0.011

atensor 16 H
-3.045 4.004 -2.162
4.004 -5.168 -1.664
-2.162 -1.664 -3.927
-0.030 0.049 -0.106
0.049 -0.056 -0.082
-0.024 -0.019 0.010

atensor 17 C
-0.462 0.347 -2.113
0.347 -0.645 -1.627

-2.113 -1.627 13.180
-0.169 0.050 -0.096
0.050 -0.196 -0.074
-0.034 -0.026 -0.011

atensor 18 H
-7.317 -2.615 0.914
-2.615 -0.893 -2.571
0.914 -2.571 -3.926
-0.082 -0.032 0.045
-0.032 -0.004 -0.126
0.010 -0.029 0.010

atensor 19 C
-0.831 -0.227 0.894
-0.227 -0.274 -2.514
0.894 -2.514 13.173
-0.223 -0.033 0.041
-0.033 -0.142 -0.114
0.014 -0.040 -0.011

atensor 20 C
-0.192 0.020 2.667
0.020 -0.910 0.072
2.667 0.072 13.165
-0.130 0.003 0.121
0.003 -0.235 0.003
0.042 0.001 -0.011

atensor 21 H
0.031 0.227 2.728
0.227 -8.237 0.074
2.728 0.074 -3.924
0.007 0.003 0.134
0.003 -0.093 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7767.637 0.084 -0.155
0.084 -7767.606 -0.401
-0.155 -0.401 -641.847
2275.747 0.000 0.004
0.000 2275.746 0.001
0.004 0.001 2268.030

orbtensor 2 H
-0.428 3.596 0.742
3.596 -9.265 -2.088
0.742 -2.088 -0.559
26.153 -4.237 -1.205
-4.237 36.563 3.389
-1.205 3.389 25.554

orbtensor 3 C
-146.772 21.911 9.274
21.911 -200.592 -26.082
9.274 -26.082 -57.730
223.644 -5.761 -4.957
-5.761 237.799 13.942
-4.957 13.942 222.147

orbtensor 4 H
-10.535 -0.312 2.215
-0.312 0.842 0.061
2.215 0.061 -0.559
38.060 0.368 -3.595
0.368 24.657 -0.099

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-3.595   -0.099   25.554

orbtensor 5 C
-208.335  -1.902   27.667
-1.902  -139.029   0.756
27.667   0.756  -57.727
239.836   0.500  -14.790
0.500  221.611  -0.406
-14.790  -0.406  222.146

orbtensor 6 H
-0.061  -3.091   0.626
-3.091  -9.631   2.125
0.626   2.125  -0.559
25.720   3.641  -1.017
3.641  36.996  -3.449
-1.017  -3.449  25.554

orbtensor 7 C
-144.515  -18.834   7.827
-18.834 -202.823  26.539
7.827   26.539 -57.728
223.057   4.951  -4.185
4.951  238.390 -14.191
-4.185  -14.191  222.147

orbtensor 8 H
-6.900   5.313  -1.827
5.313  -2.791   1.253
-1.827   1.253  -0.558
33.779  -6.260   2.966
-6.260  28.937  -2.033
2.966  -2.033  25.554

orbtensor 9 C
-186.171  32.372  -22.823
32.372 -161.140  15.643
-22.823  15.643 -57.729
234.012  -8.511  12.204
-8.511  227.430  -8.365
12.204  -8.365  222.148

orbtensor 10 H
-6.306  -5.506  -1.756
-5.506  -3.385  -1.351
-1.756  -1.351  -0.558
33.079   6.487   2.851
6.487  29.637   2.193
2.851   2.193  25.554

orbtensor 11 C
-182.556  -33.543  -21.934
-33.543 -164.770  -16.878
-21.934 -16.878  -57.729
233.061   8.820   11.727
8.820  228.381   9.023
11.727   9.023  222.148

orbtensor 12 H
-0.061  -3.090  -0.627
-3.090  -9.630  -2.126
-0.627  -2.126  -0.559
25.721   3.641   1.017
3.641  36.996   3.451
1.017   3.451  25.555

orbtensor 13 C

```

-144.497	-18.825	-7.822
-18.825	-202.808	-26.568
-7.822	-26.568	-57.733
223.054	4.951	4.183
4.951	238.384	14.195
4.183	14.195	222.151

orbtensor 14 H

-6.901	5.313	1.829
5.313	-2.792	-1.254
1.829	-1.254	-0.559
33.779	-6.259	-2.968
-6.259	28.938	2.034
-2.968	2.034	25.554

orbtensor 15 C

-186.207	32.363	22.857
32.363	-161.163	-15.666
22.857	-15.666	-57.736
234.014	-8.510	-12.207
-8.510	227.431	8.365
-12.207	8.365	222.149

orbtensor 16 H

-6.307	-5.507	1.757
-5.507	-3.387	1.352
1.757	1.352	-0.559
33.079	6.487	-2.851
6.487	29.639	-2.193
-2.851	-2.193	25.554

orbtensor 17 C

-182.595	-33.540	21.960
-33.540	-164.803	16.882
21.960	16.882	-57.727
233.062	8.821	-11.728
8.821	228.386	-9.022
-11.728	-9.022	222.145

orbtensor 18 H

-0.428	3.596	-0.743
3.596	-9.264	2.088
-0.743	2.088	-0.559
26.153	-4.237	1.204
-4.237	36.564	-3.388
1.204	-3.388	25.554

orbtensor 19 C

-146.756	21.903	-9.265
21.903	-200.597	26.083
-9.265	26.083	-57.725
223.643	-5.762	4.954
-5.762	237.799	-13.942
4.954	-13.942	222.144

orbtensor 20 C

-208.302	-1.897	-27.667
-1.897	-138.992	-0.764
-27.667	-0.764	-57.728
239.831	0.499	14.791
0.499	221.606	0.405
14.791	0.405	222.147

orbtensor 21 H

-10.533	-0.312	-2.215
-0.312	0.842	-0.061
-2.215	-0.061	-0.559

```

38.059    0.368    3.595
0.368    24.657    0.098
3.595    0.098    25.554

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gtensor (ppt)
-0.046    0.000    0.000
 0.000   -0.046    0.000
 0.000    0.000   -0.208
42.117   -0.001    0.006
-0.001   42.116    0.003
 0.006    0.003    1.051

```

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averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

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Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.9363	-3119.18900	35176.34905	228.61360	35404.96265	32285.77365
2	H	-4.0717	26.00600	291.81200	0.07494	291.88694	317.89294
3	C	3.8977	92.83200	-1110.68920	17.87181	-1092.81739	-999.98539
4	H	-4.0717	26.00633	291.81200	0.07538	291.88737	317.89371
5	C	3.8977	92.83400	-1110.68920	17.87358	-1092.81563	-999.98163
6	H	-4.0707	26.00633	291.74033	0.07541	291.81575	317.82208
7	C	3.8973	92.84267	-1110.59422	17.86617	-1092.72804	-999.88538
8	H	-4.0693	26.00700	291.64477	0.07453	291.71930	317.72630
9	C	3.8950	92.85000	-1109.92930	17.85701	-1092.07229	-999.22229
10	H	-4.0697	26.00700	291.66866	0.07466	291.74333	317.75033
11	C	3.8947	92.84500	-1109.83432	17.86073	-1091.97359	-999.12859
12	H	-4.0690	26.00733	291.62088	0.07497	291.69585	317.70319
13	C	3.8960	92.85033	-1110.21427	17.85675	-1092.35752	-999.50718
14	H	-4.0720	26.00633	291.83589	0.07528	291.91117	317.91751
15	C	3.8980	92.82933	-1110.78419	17.87411	-1092.91008	-1000.08075
16	H	-4.0720	26.00633	291.83589	0.07570	291.91159	317.91792
17	C	3.8990	92.82267	-1111.06915	17.87890	-1093.19026	-1000.36759
18	H	-4.0707	26.00667	291.74033	0.07505	291.81538	317.82204
19	C	3.8973	92.83600	-1110.59422	17.86709	-1092.72713	-999.89113
20	C	3.8957	92.85400	-1110.11928	17.85309	-1092.26618	-999.41218
21	H	-4.0687	26.00667	291.59699	0.07457	291.67156	317.67823
13C Average		3.8968	92.83960	-1110.45173	17.86592	-1092.58581	-999.74621
1H Average		-4.0705	26.00660	291.73077	0.07505	291.80582	317.81242

```

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3NiCp2-STO-PBE-Neese
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
91.492 0.000 0.011
0.000 91.492 0.006
0.011 0.006 4.436
-26.459 0.000 -0.003
0.000 -26.459 -0.002
-0.003 -0.002 -2.693

```

```

atensor 2 H
-7.318 -2.614 -0.914
-2.614 -0.894 2.571
-0.914 2.571 -3.927
-0.082 -0.032 -0.045
-0.032 -0.004 0.126
-0.010 0.029 0.010

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atensor 3 C

```

-0.832 -0.227 -0.894
-0.227 -0.275 2.514
-0.894 2.514 13.176
-0.223 -0.033 -0.041
-0.033 -0.142 0.114
-0.014 0.040 -0.011

atensor 4 H
0.030 0.227 -2.728
0.227 -8.242 -0.075
-2.728 -0.075 -3.927
0.007 0.003 -0.134
0.003 -0.093 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.195 0.020 -2.667
0.020 -0.912 -0.073
-2.667 -0.073 13.176
-0.130 0.003 -0.121
0.003 -0.235 -0.003
-0.042 -0.001 -0.011

atensor 6 H
-7.584 2.247 -0.772
2.247 -0.626 -2.617
-0.772 -2.618 -3.926
-0.085 0.027 -0.038
0.027 -0.001 -0.128
-0.009 -0.030 0.010

atensor 7 C
-0.854 0.195 -0.754
0.195 -0.250 -2.559
-0.754 -2.560 13.172
-0.226 0.028 -0.034
0.028 -0.139 -0.116
-0.012 -0.041 -0.011

atensor 8 H
-2.610 -3.862 2.251
-3.862 -5.597 -1.543
2.251 -1.543 -3.925
-0.025 -0.047 0.110
-0.047 -0.061 -0.076
0.025 -0.017 0.010

atensor 9 C
-0.423 -0.335 2.201
-0.335 -0.682 -1.509
2.201 -1.509 13.166
-0.164 -0.049 0.100
-0.049 -0.201 -0.069
0.035 -0.024 -0.011

atensor 10 H
-3.042 4.003 2.163
4.003 -5.166 1.664
2.163 1.664 -3.925
-0.030 0.049 0.106
0.049 -0.056 0.082
0.024 0.019 0.010

atensor 11 C
-0.462 0.347 2.115
0.347 -0.646 1.626
2.115 1.626 13.168

-0.169 0.051 0.096
0.051 -0.196 0.074
0.034 0.026 -0.011

atensor 12 H
-7.581 2.247 0.772
2.247 -0.626 2.618
0.772 2.618 -3.924
-0.085 0.027 0.038
0.027 -0.001 0.128
0.009 0.030 0.010

atensor 13 C
-0.853 0.195 0.755
0.195 -0.251 2.557
0.755 2.557 13.167
-0.226 0.028 0.034
0.028 -0.138 0.116
0.012 0.041 -0.011

atensor 14 H
-2.613 -3.863 -2.251
-3.863 -5.600 1.543
-2.251 1.543 -3.927
-0.025 -0.047 -0.110
-0.047 -0.061 0.076
-0.025 0.017 0.010

atensor 15 C
-0.424 -0.335 -2.199
-0.335 -0.683 1.506
-2.199 1.507 13.177
-0.164 -0.049 -0.100
-0.049 -0.201 0.069
-0.035 0.024 -0.011

atensor 16 H
-3.045 4.004 -2.162
4.004 -5.168 -1.664
-2.162 -1.664 -3.927
-0.030 0.049 -0.106
0.049 -0.056 -0.082
-0.024 -0.019 0.010

atensor 17 C
-0.462 0.347 -2.113
0.347 -0.645 -1.627
-2.113 -1.627 13.180
-0.169 0.050 -0.096
0.050 -0.196 -0.074
-0.034 -0.026 -0.011

atensor 18 H
-7.317 -2.615 0.914
-2.615 -0.893 -2.571
0.914 -2.571 -3.926
-0.082 -0.032 0.045
-0.032 -0.004 -0.126
0.010 -0.029 0.010

atensor 19 C
-0.831 -0.227 0.894
-0.227 -0.274 -2.514
0.894 -2.514 13.173
-0.223 -0.033 0.041
-0.033 -0.142 -0.114
0.014 -0.040 -0.011

atensor 20 C
-0.192 0.020 2.667
0.020 -0.910 0.072
2.667 0.072 13.165
-0.130 0.003 0.121
0.003 -0.235 0.003
0.042 0.001 -0.011

atensor 21 H
0.031 0.227 2.728
0.227 -8.237 0.074
2.728 0.074 -3.924
0.007 0.003 0.134
0.003 -0.093 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7767.637 0.084 -0.155
0.084 -7767.606 -0.401
-0.155 -0.401 -641.847
2275.747 0.000 0.004
0.000 2275.746 0.001
0.004 0.001 2268.030

orbtensor 2 H
-0.428 3.596 0.742
3.596 -9.265 -2.088
0.742 -2.088 -0.559
26.153 -4.237 -1.205
-4.237 36.563 3.389
-1.205 3.389 25.554

orbtensor 3 C
-146.772 21.911 9.274
21.911 -200.592 -26.082
9.274 -26.082 -57.730
223.644 -5.761 -4.957
-5.761 237.799 13.942
-4.957 13.942 222.147

orbtensor 4 H
-10.535 -0.312 2.215
-0.312 0.842 0.061
2.215 0.061 -0.559
38.060 0.368 -3.595
0.368 24.657 -0.099
-3.595 -0.099 25.554

orbtensor 5 C
-208.335 -1.902 27.667
-1.902 -139.029 0.756
27.667 0.756 -57.727
239.836 0.500 -14.790
0.500 221.611 -0.406
-14.790 -0.406 222.146

orbtensor 6 H
-0.061 -3.091 0.626
-3.091 -9.631 2.125
0.626 2.125 -0.559
25.720 3.641 -1.017
3.641 36.996 -3.449
-1.017 -3.449 25.554

orbtensor 7 C
-144.515 -18.834 7.827

-18.834	-202.823	26.539
7.827	26.539	-57.728
223.057	4.951	-4.185
4.951	238.390	-14.191
-4.185	-14.191	222.147

orbtensor 8 H

-6.900	5.313	-1.827
5.313	-2.791	1.253
-1.827	1.253	-0.558
33.779	-6.260	2.966
-6.260	28.937	-2.033
2.966	-2.033	25.554

orbtensor 9 C

-186.171	32.372	-22.823
32.372	-161.140	15.643
-22.823	15.643	-57.729
234.012	-8.511	12.204
-8.511	227.430	-8.365
12.204	-8.365	222.148

orbtensor 10 H

-6.306	-5.506	-1.756
-5.506	-3.385	-1.351
-1.756	-1.351	-0.558
33.079	6.487	2.851
6.487	29.637	2.193
2.851	2.193	25.554

orbtensor 11 C

-182.556	-33.543	-21.934
-33.543	-164.770	-16.878
-21.934	-16.878	-57.729
233.061	8.820	11.727
8.820	228.381	9.023
11.727	9.023	222.148

orbtensor 12 H

-0.061	-3.090	-0.627
-3.090	-9.630	-2.126
-0.627	-2.126	-0.559
25.721	3.641	1.017
3.641	36.996	3.451
1.017	3.451	25.555

orbtensor 13 C

-144.497	-18.825	-7.822
-18.825	-202.808	-26.568
-7.822	-26.568	-57.733
223.054	4.951	4.183
4.951	238.384	14.195
4.183	14.195	222.151

orbtensor 14 H

-6.901	5.313	1.829
5.313	-2.792	-1.254
1.829	-1.254	-0.559
33.779	-6.259	-2.968
-6.259	28.938	2.034
-2.968	2.034	25.554

orbtensor 15 C

-186.207	32.363	22.857
32.363	-161.163	-15.666
22.857	-15.666	-57.736
234.014	-8.510	-12.207

-8.510 227.431 8.365
-12.207 8.365 222.149

orbtensor 16 H
-6.307 -5.507 1.757
-5.507 -3.387 1.352
1.757 1.352 -0.559
33.079 6.487 -2.851
6.487 29.639 -2.193
-2.851 -2.193 25.554

orbtensor 17 C
-182.595 -33.540 21.960
-33.540 -164.803 16.882
21.960 16.882 -57.727
233.062 8.821 -11.728
8.821 228.386 -9.022
-11.728 -9.022 222.145

orbtensor 18 H
-0.428 3.596 -0.743
3.596 -9.264 2.088
-0.743 2.088 -0.559
26.153 -4.237 1.204
-4.237 36.564 -3.388
1.204 -3.388 25.554

orbtensor 19 C
-146.756 21.903 -9.265
21.903 -200.597 26.083
-9.265 26.083 -57.725
223.643 -5.762 4.954
-5.762 237.799 -13.942
4.954 -13.942 222.144

orbtensor 20 C
-208.302 -1.897 -27.667
-1.897 -138.992 -0.764
-27.667 -0.764 -57.728
239.831 0.499 14.791
0.499 221.606 0.405
14.791 0.405 222.147

orbtensor 21 H
-10.533 -0.312 -2.215
-0.312 0.842 -0.061
-2.215 -0.061 -0.559
38.059 0.368 3.595
0.368 24.657 0.098
3.595 0.098 25.554

gtensor (ppt)
-0.046 0.000 0.000
0.000 -0.046 0.000
0.000 0.000 -0.208
42.117 -0.001 0.006
-0.001 42.116 0.003
0.006 0.003 1.051

zfstensor (cm-1)
-1.599606 0.000031 0.002127
0.000031 -1.599612 0.000054
0.002127 0.000054 3.199218

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.9363	-3119.18900	35177.13443	358.16444	35535.29887	32416.10987
2	H	-4.0717	26.00600	291.81851	0.11722	291.93574	317.94174
3	C	3.8977	92.83200	-1110.71400	27.99871	-1082.71530	-989.88330
4	H	-4.0717	26.00633	291.81851	0.11720	291.93571	317.94205
5	C	3.8977	92.83400	-1110.71400	27.99863	-1082.71537	-989.88137
6	H	-4.0707	26.00633	291.74684	0.11772	291.86456	317.87090
7	C	3.8973	92.84267	-1110.61901	27.98908	-1082.62994	-989.78727
8	H	-4.0693	26.00700	291.65128	0.11749	291.76878	317.77578
9	C	3.8950	92.85000	-1109.95408	27.97889	-1081.97520	-989.12520
10	H	-4.0697	26.00700	291.67517	0.11775	291.79292	317.79992
11	C	3.8947	92.84500	-1109.85909	27.98516	-1081.87393	-989.02893
12	H	-4.0690	26.00733	291.62739	0.11779	291.74519	317.75252
13	C	3.8960	92.85033	-1110.23905	27.97729	-1082.26176	-989.41143
14	H	-4.0720	26.00633	291.84241	0.11731	291.95972	317.96605
15	C	3.8980	92.82933	-1110.80899	28.00040	-1082.80859	-989.97926
16	H	-4.0720	26.00633	291.84241	0.11776	291.96016	317.96650
17	C	3.8990	92.82267	-1111.09396	28.00739	-1083.08657	-990.26391
18	H	-4.0707	26.00667	291.74684	0.11776	291.86460	317.87127
19	C	3.8973	92.83600	-1110.61901	27.99273	-1082.62628	-989.79028
20	C	3.8957	92.85400	-1110.14406	27.97367	-1082.17040	-989.31640
21	H	-4.0687	26.00667	291.60350	0.11777	291.72128	317.72794
13C Average		3.8968	92.83960	-1110.47653	27.99019	-1082.48633	-989.64673
1H Average		-4.0705	26.00660	291.73729	0.11758	291.85487	317.86147

3NiCp2-STO-PBE-ORCA

Temperature: 298

Spin: 1

atensor 1 Ni

91.492 0.000 0.011
0.000 91.492 0.006
0.011 0.006 4.436
-26.459 0.000 -0.003
0.000 -26.459 -0.002
-0.003 -0.002 -2.693

atensor 2 H

-7.318 -2.614 -0.914
-2.614 -0.894 2.571
-0.914 2.571 -3.927
-0.082 -0.032 -0.045
-0.032 -0.004 0.126
-0.010 0.029 0.010

atensor 3 C

-0.832 -0.227 -0.894
-0.227 -0.275 2.514
-0.894 2.514 13.176
-0.223 -0.033 -0.041
-0.033 -0.142 0.114
-0.014 0.040 -0.011

atensor 4 H

0.030 0.227 -2.728
0.227 -8.242 -0.075
-2.728 -0.075 -3.927
0.007 0.003 -0.134
0.003 -0.093 -0.004
-0.031 -0.001 0.010

atensor 5 C
-0.195 0.020 -2.667
0.020 -0.912 -0.073
-2.667 -0.073 13.176
-0.130 0.003 -0.121
0.003 -0.235 -0.003
-0.042 -0.001 -0.011

atensor 6 H
-7.584 2.247 -0.772
2.247 -0.626 -2.617
-0.772 -2.618 -3.926
-0.085 0.027 -0.038
0.027 -0.001 -0.128
-0.009 -0.030 0.010

atensor 7 C
-0.854 0.195 -0.754
0.195 -0.250 -2.559
-0.754 -2.560 13.172
-0.226 0.028 -0.034
0.028 -0.139 -0.116
-0.012 -0.041 -0.011

atensor 8 H
-2.610 -3.862 2.251
-3.862 -5.597 -1.543
2.251 -1.543 -3.925
-0.025 -0.047 0.110
-0.047 -0.061 -0.076
0.025 -0.017 0.010

atensor 9 C
-0.423 -0.335 2.201
-0.335 -0.682 -1.509
2.201 -1.509 13.166
-0.164 -0.049 0.100
-0.049 -0.201 -0.069
0.035 -0.024 -0.011

atensor 10 H
-3.042 4.003 2.163
4.003 -5.166 1.664
2.163 1.664 -3.925
-0.030 0.049 0.106
0.049 -0.056 0.082
0.024 0.019 0.010

atensor 11 C
-0.462 0.347 2.115
0.347 -0.646 1.626
2.115 1.626 13.168
-0.169 0.051 0.096
0.051 -0.196 0.074
0.034 0.026 -0.011

atensor 12 H
-7.581 2.247 0.772
2.247 -0.626 2.618
0.772 2.618 -3.924
-0.085 0.027 0.038
0.027 -0.001 0.128
0.009 0.030 0.010

atensor 13 C
-0.853 0.195 0.755
0.195 -0.251 2.557

0.755 2.557 13.167
-0.226 0.028 0.034
0.028 -0.138 0.116
0.012 0.041 -0.011

atensor 14 H
-2.613 -3.863 -2.251
-3.863 -5.600 1.543
-2.251 1.543 -3.927
-0.025 -0.047 -0.110
-0.047 -0.061 0.076
-0.025 0.017 0.010

atensor 15 C
-0.424 -0.335 -2.199
-0.335 -0.683 1.506
-2.199 1.507 13.177
-0.164 -0.049 -0.100
-0.049 -0.201 0.069
-0.035 0.024 -0.011

atensor 16 H
-3.045 4.004 -2.162
4.004 -5.168 -1.664
-2.162 -1.664 -3.927
-0.030 0.049 -0.106
0.049 -0.056 -0.082
-0.024 -0.019 0.010

atensor 17 C
-0.462 0.347 -2.113
0.347 -0.645 -1.627
-2.113 -1.627 13.180
-0.169 0.050 -0.096
0.050 -0.196 -0.074
-0.034 -0.026 -0.011

atensor 18 H
-7.317 -2.615 0.914
-2.615 -0.893 -2.571
0.914 -2.571 -3.926
-0.082 -0.032 0.045
-0.032 -0.004 -0.126
0.010 -0.029 0.010

atensor 19 C
-0.831 -0.227 0.894
-0.227 -0.274 -2.514
0.894 -2.514 13.173
-0.223 -0.033 0.041
-0.033 -0.142 -0.114
0.014 -0.040 -0.011

atensor 20 C
-0.192 0.020 2.667
0.020 -0.910 0.072
2.667 0.072 13.165
-0.130 0.003 0.121
0.003 -0.235 0.003
0.042 0.001 -0.011

atensor 21 H
0.031 0.227 2.728
0.227 -8.237 0.074
2.728 0.074 -3.924
0.007 0.003 0.134
0.003 -0.093 0.004

0.031 0.001 0.010

orbtensor 1 Ni

-7767.637	0.084	-0.155
0.084	-7767.606	-0.401
-0.155	-0.401	-641.847
2275.747	0.000	0.004
0.000	2275.746	0.001
0.004	0.001	2268.030

orbtensor 2 H

-0.428	3.596	0.742
3.596	-9.265	-2.088
0.742	-2.088	-0.559
26.153	-4.237	-1.205
-4.237	36.563	3.389
-1.205	3.389	25.554

orbtensor 3 C

-146.772	21.911	9.274
21.911	-200.592	-26.082
9.274	-26.082	-57.730
223.644	-5.761	-4.957
-5.761	237.799	13.942
-4.957	13.942	222.147

orbtensor 4 H

-10.535	-0.312	2.215
-0.312	0.842	0.061
2.215	0.061	-0.559
38.060	0.368	-3.595
0.368	24.657	-0.099
-3.595	-0.099	25.554

orbtensor 5 C

-208.335	-1.902	27.667
-1.902	-139.029	0.756
27.667	0.756	-57.727
239.836	0.500	-14.790
0.500	221.611	-0.406
-14.790	-0.406	222.146

orbtensor 6 H

-0.061	-3.091	0.626
-3.091	-9.631	2.125
0.626	2.125	-0.559
25.720	3.641	-1.017
3.641	36.996	-3.449
-1.017	-3.449	25.554

orbtensor 7 C

-144.515	-18.834	7.827
-18.834	-202.823	26.539
7.827	26.539	-57.728
223.057	4.951	-4.185
4.951	238.390	-14.191
-4.185	-14.191	222.147

orbtensor 8 H

-6.900	5.313	-1.827
5.313	-2.791	1.253
-1.827	1.253	-0.558
33.779	-6.260	2.966
-6.260	28.937	-2.033
2.966	-2.033	25.554

orbtensor 9 C

-186.171	32.372	-22.823
32.372	-161.140	15.643
-22.823	15.643	-57.729
234.012	-8.511	12.204
-8.511	227.430	-8.365
12.204	-8.365	222.148

orbtensor 10 H

-6.306	-5.506	-1.756
-5.506	-3.385	-1.351
-1.756	-1.351	-0.558
33.079	6.487	2.851
6.487	29.637	2.193
2.851	2.193	25.554

orbtensor 11 C

-182.556	-33.543	-21.934
-33.543	-164.770	-16.878
-21.934	-16.878	-57.729
233.061	8.820	11.727
8.820	228.381	9.023
11.727	9.023	222.148

orbtensor 12 H

-0.061	-3.090	-0.627
-3.090	-9.630	-2.126
-0.627	-2.126	-0.559
25.721	3.641	1.017
3.641	36.996	3.451
1.017	3.451	25.555

orbtensor 13 C

-144.497	-18.825	-7.822
-18.825	-202.808	-26.568
-7.822	-26.568	-57.733
223.054	4.951	4.183
4.951	238.384	14.195
4.183	14.195	222.151

orbtensor 14 H

-6.901	5.313	1.829
5.313	-2.792	-1.254
1.829	-1.254	-0.559
33.779	-6.259	-2.968
-6.259	28.938	2.034
-2.968	2.034	25.554

orbtensor 15 C

-186.207	32.363	22.857
32.363	-161.163	-15.666
22.857	-15.666	-57.736
234.014	-8.510	-12.207
-8.510	227.431	8.365
-12.207	8.365	222.149

orbtensor 16 H

-6.307	-5.507	1.757
-5.507	-3.387	1.352
1.757	1.352	-0.559
33.079	6.487	-2.851
6.487	29.639	-2.193
-2.851	-2.193	25.554

orbtensor 17 C

-182.595	-33.540	21.960
-33.540	-164.803	16.882
21.960	16.882	-57.727

233.062 8.821 -11.728
 8.821 228.386 -9.022
 -11.728 -9.022 222.145

orbtensor 18 H
 -0.428 3.596 -0.743
 3.596 -9.264 2.088
 -0.743 2.088 -0.559
 26.153 -4.237 1.204
 -4.237 36.564 -3.388
 1.204 -3.388 25.554

orbtensor 19 C
 -146.756 21.903 -9.265
 21.903 -200.597 26.083
 -9.265 26.083 -57.725
 223.643 -5.762 4.954
 -5.762 237.799 -13.942
 4.954 -13.942 222.144

orbtensor 20 C
 -208.302 -1.897 -27.667
 -1.897 -138.992 -0.764
 -27.667 -0.764 -57.728
 239.831 0.499 14.791
 0.499 221.606 0.405
 14.791 0.405 222.147

orbtensor 21 H
 -10.533 -0.312 -2.215
 -0.312 0.842 -0.061
 -2.215 -0.061 -0.559
 38.059 0.368 3.595
 0.368 24.657 0.098
 3.595 0.098 25.554

gtensor (ppt)
 -0.046 0.000 0.000
 0.000 -0.046 0.000
 0.000 0.000 -0.208
 42.117 -0.001 0.006
 -0.001 42.116 0.003
 0.006 0.003 1.051

zfstensor (cm-1)
 44.296232 0.000277 0.002021
 0.000277 44.295565 -0.000105
 0.002021 -0.000105 48.809312

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.9363	-3119.18900	35177.14684	350.46034	35527.60718	32408.41818
2	H	-4.0717	26.00600	291.81862	0.11446	291.93308	317.93908
3	C	3.8977	92.83200	-1110.71439	27.39621	-1083.31818	-990.48618
4	H	-4.0717	26.00633	291.81862	0.11487	291.93349	317.93983
5	C	3.8977	92.83400	-1110.71439	27.39656	-1083.31783	-990.48383
6	H	-4.0707	26.00633	291.74695	0.11518	291.86213	317.86846
7	C	3.8973	92.84267	-1110.61940	27.38724	-1083.23216	-990.38949
8	H	-4.0693	26.00700	291.65139	0.11492	291.76630	317.77330
9	C	3.8950	92.85000	-1109.95448	27.37707	-1082.57740	-989.72740
10	H	-4.0697	26.00700	291.67528	0.11532	291.79059	317.79759

11	C	3.8947	92.84500	-1109.85949	27.38305	-1082.47644	-989.63144
12	H	-4.0690	26.00733	291.62750	0.11513	291.74263	317.74996
13	C	3.8960	92.85033	-1110.23944	27.37524	-1082.86421	-990.01387
14	H	-4.0720	26.00633	291.84251	0.11473	291.95723	317.96357
15	C	3.8980	92.82933	-1110.80938	27.39805	-1083.41133	-990.58199
16	H	-4.0720	26.00633	291.84251	0.11544	291.95795	317.96428
17	C	3.8990	92.82267	-1111.09435	27.40523	-1083.68912	-990.86646
18	H	-4.0707	26.00667	291.74695	0.11507	291.86202	317.86868
19	C	3.8973	92.83600	-1110.61940	27.39070	-1083.22871	-990.39271
20	C	3.8957	92.85400	-1110.14446	27.37190	-1082.77255	-989.91855
21	H	-4.0687	26.00667	291.60361	0.11538	291.71898	317.72565
13C Average		3.8968	92.83960	-1110.47692	27.38813	-1083.08879	-990.24919
1H Average		-4.0705	26.00660	291.73739	0.11505	291.85244	317.85904

=====

3NiCp2-STO-PBE-Pederson

Temperature: 298

Spin: 1

atensor 1 Ni

91.492 0.000 0.011
0.000 91.492 0.006
0.011 0.006 4.436
-26.459 0.000 -0.003
0.000 -26.459 -0.002
-0.003 -0.002 -2.693

atensor 2 H

-7.318 -2.614 -0.914
-2.614 -0.894 2.571
-0.914 2.571 -3.927
-0.082 -0.032 -0.045
-0.032 -0.004 0.126
-0.010 0.029 0.010

atensor 3 C

-0.832 -0.227 -0.894
-0.227 -0.275 2.514
-0.894 2.514 13.176
-0.223 -0.033 -0.041
-0.033 -0.142 0.114
-0.014 0.040 -0.011

atensor 4 H

0.030 0.227 -2.728
0.227 -8.242 -0.075
-2.728 -0.075 -3.927
0.007 0.003 -0.134
0.003 -0.093 -0.004
-0.031 -0.001 0.010

atensor 5 C

-0.195 0.020 -2.667
0.020 -0.912 -0.073
-2.667 -0.073 13.176
-0.130 0.003 -0.121
0.003 -0.235 -0.003
-0.042 -0.001 -0.011

atensor 6 H

-7.584 2.247 -0.772
2.247 -0.626 -2.617
-0.772 -2.618 -3.926
-0.085 0.027 -0.038
0.027 -0.001 -0.128
-0.009 -0.030 0.010

atensor 7 C
-0.854 0.195 -0.754
0.195 -0.250 -2.559
-0.754 -2.560 13.172
-0.226 0.028 -0.034
0.028 -0.139 -0.116
-0.012 -0.041 -0.011

atensor 8 H
-2.610 -3.862 2.251
-3.862 -5.597 -1.543
2.251 -1.543 -3.925
-0.025 -0.047 0.110
-0.047 -0.061 -0.076
0.025 -0.017 0.010

atensor 9 C
-0.423 -0.335 2.201
-0.335 -0.682 -1.509
2.201 -1.509 13.166
-0.164 -0.049 0.100
-0.049 -0.201 -0.069
0.035 -0.024 -0.011

atensor 10 H
-3.042 4.003 2.163
4.003 -5.166 1.664
2.163 1.664 -3.925
-0.030 0.049 0.106
0.049 -0.056 0.082
0.024 0.019 0.010

atensor 11 C
-0.462 0.347 2.115
0.347 -0.646 1.626
2.115 1.626 13.168
-0.169 0.051 0.096
0.051 -0.196 0.074
0.034 0.026 -0.011

atensor 12 H
-7.581 2.247 0.772
2.247 -0.626 2.618
0.772 2.618 -3.924
-0.085 0.027 0.038
0.027 -0.001 0.128
0.009 0.030 0.010

atensor 13 C
-0.853 0.195 0.755
0.195 -0.251 2.557
0.755 2.557 13.167
-0.226 0.028 0.034
0.028 -0.138 0.116
0.012 0.041 -0.011

atensor 14 H
-2.613 -3.863 -2.251
-3.863 -5.600 1.543
-2.251 1.543 -3.927
-0.025 -0.047 -0.110
-0.047 -0.061 0.076
-0.025 0.017 0.010

atensor 15 C
-0.424 -0.335 -2.199

-0.335 -0.683 1.506
-2.199 1.507 13.177
-0.164 -0.049 -0.100
-0.049 -0.201 0.069
-0.035 0.024 -0.011

atensor 16 H
-3.045 4.004 -2.162
4.004 -5.168 -1.664
-2.162 -1.664 -3.927
-0.030 0.049 -0.106
0.049 -0.056 -0.082
-0.024 -0.019 0.010

atensor 17 C
-0.462 0.347 -2.113
0.347 -0.645 -1.627
-2.113 -1.627 13.180
-0.169 0.050 -0.096
0.050 -0.196 -0.074
-0.034 -0.026 -0.011

atensor 18 H
-7.317 -2.615 0.914
-2.615 -0.893 -2.571
0.914 -2.571 -3.926
-0.082 -0.032 0.045
-0.032 -0.004 -0.126
0.010 -0.029 0.010

atensor 19 C
-0.831 -0.227 0.894
-0.227 -0.274 -2.514
0.894 -2.514 13.173
-0.223 -0.033 0.041
-0.033 -0.142 -0.114
0.014 -0.040 -0.011

atensor 20 C
-0.192 0.020 2.667
0.020 -0.910 0.072
2.667 0.072 13.165
-0.130 0.003 0.121
0.003 -0.235 0.003
0.042 0.001 -0.011

atensor 21 H
0.031 0.227 2.728
0.227 -8.237 0.074
2.728 0.074 -3.924
0.007 0.003 0.134
0.003 -0.093 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7767.637 0.084 -0.155
0.084 -7767.606 -0.401
-0.155 -0.401 -641.847
2275.747 0.000 0.004
0.000 2275.746 0.001
0.004 0.001 2268.030

orbtensor 2 H
-0.428 3.596 0.742
3.596 -9.265 -2.088
0.742 -2.088 -0.559
26.153 -4.237 -1.205

```

-4.237    36.563    3.389
-1.205    3.389    25.554

orbtensor 3 C
-146.772   21.911    9.274
21.911  -200.592  -26.082
9.274   -26.082  -57.730
223.644   -5.761   -4.957
-5.761   237.799   13.942
-4.957   13.942   222.147

orbtensor 4 H
-10.535   -0.312    2.215
-0.312    0.842    0.061
2.215     0.061   -0.559
38.060    0.368   -3.595
0.368    24.657   -0.099
-3.595   -0.099   25.554

orbtensor 5 C
-208.335  -1.902    27.667
-1.902  -139.029    0.756
27.667    0.756  -57.727
239.836    0.500  -14.790
0.500   221.611   -0.406
-14.790   -0.406   222.146

orbtensor 6 H
-0.061   -3.091    0.626
-3.091   -9.631    2.125
0.626    2.125   -0.559
25.720    3.641   -1.017
3.641   36.996   -3.449
-1.017   -3.449   25.554

orbtensor 7 C
-144.515  -18.834    7.827
-18.834  -202.823   26.539
7.827   26.539  -57.728
223.057    4.951   -4.185
4.951   238.390  -14.191
-4.185  -14.191   222.147

orbtensor 8 H
-6.900    5.313   -1.827
5.313   -2.791    1.253
-1.827    1.253   -0.558
33.779   -6.260    2.966
-6.260   28.937   -2.033
2.966   -2.033   25.554

orbtensor 9 C
-186.171   32.372  -22.823
32.372  -161.140   15.643
-22.823   15.643  -57.729
234.012   -8.511   12.204
-8.511   227.430   -8.365
12.204   -8.365   222.148

orbtensor 10 H
-6.306   -5.506   -1.756
-5.506   -3.385   -1.351
-1.756   -1.351   -0.558
33.079    6.487    2.851
6.487   29.637    2.193
2.851    2.193   25.554

```

orbtensor 11 C
-182.556 -33.543 -21.934
-33.543 -164.770 -16.878
-21.934 -16.878 -57.729
233.061 8.820 11.727
8.820 228.381 9.023
11.727 9.023 222.148

orbtensor 12 H
-0.061 -3.090 -0.627
-3.090 -9.630 -2.126
-0.627 -2.126 -0.559
25.721 3.641 1.017
3.641 36.996 3.451
1.017 3.451 25.555

orbtensor 13 C
-144.497 -18.825 -7.822
-18.825 -202.808 -26.568
-7.822 -26.568 -57.733
223.054 4.951 4.183
4.951 238.384 14.195
4.183 14.195 222.151

orbtensor 14 H
-6.901 5.313 1.829
5.313 -2.792 -1.254
1.829 -1.254 -0.559
33.779 -6.259 -2.968
-6.259 28.938 2.034
-2.968 2.034 25.554

orbtensor 15 C
-186.207 32.363 22.857
32.363 -161.163 -15.666
22.857 -15.666 -57.736
234.014 -8.510 -12.207
-8.510 227.431 8.365
-12.207 8.365 222.149

orbtensor 16 H
-6.307 -5.507 1.757
-5.507 -3.387 1.352
1.757 1.352 -0.559
33.079 6.487 -2.851
6.487 29.639 -2.193
-2.851 -2.193 25.554

orbtensor 17 C
-182.595 -33.540 21.960
-33.540 -164.803 16.882
21.960 16.882 -57.727
233.062 8.821 -11.728
8.821 228.386 -9.022
-11.728 -9.022 222.145

orbtensor 18 H
-0.428 3.596 -0.743
3.596 -9.264 2.088
-0.743 2.088 -0.559
26.153 -4.237 1.204
-4.237 36.564 -3.388
1.204 -3.388 25.554

orbtensor 19 C
-146.756 21.903 -9.265
21.903 -200.597 26.083

```

-9.265    26.083   -57.725
223.643   -5.762    4.954
-5.762   237.799   -13.942
4.954   -13.942   222.144

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orbtensor 20 C
-208.302  -1.897  -27.667
-1.897  -138.992  -0.764
-27.667  -0.764  -57.728
239.831   0.499  14.791
0.499   221.606   0.405
14.791   0.405   222.147

```

```

orbtensor 21 H
-10.533  -0.312  -2.215
-0.312   0.842  -0.061
-2.215  -0.061  -0.559
38.059   0.368   3.595
0.368   24.657   0.098
3.595   0.098   25.554

```

```

gtensor (ppt)
-0.046   0.000   0.000
 0.000  -0.046   0.000
 0.000   0.000  -0.208
42.117  -0.001   0.006
-0.001  42.116   0.003
 0.006   0.003   1.051

```

```

zfstensor (cm-1)
-2.990515  -0.000067   0.000527
-0.000067  -2.990489   0.000429
 0.000527   0.000429   5.981004

```

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averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.9363	-3119.18900	35176.09314	470.77318	35646.86632	32527.67732
2	H	-4.0717	26.00600	291.80988	0.15450	291.96438	317.97038
3	C	3.8977	92.83200	-1110.68112	36.80311	-1073.87802	-981.04602
4	H	-4.0717	26.00633	291.80988	0.15465	291.96453	317.97086
5	C	3.8977	92.83400	-1110.68112	36.80389	-1073.87723	-981.04323
6	H	-4.0707	26.00633	291.73821	0.15468	291.89289	317.89922
7	C	3.8973	92.84267	-1110.58614	36.78897	-1073.79717	-980.95450
8	H	-4.0693	26.00700	291.64265	0.15391	291.79656	317.80356
9	C	3.8950	92.85000	-1109.92123	36.77328	-1073.14795	-980.29795
10	H	-4.0697	26.00700	291.66654	0.15431	291.82085	317.82785
11	C	3.8947	92.84500	-1109.82624	36.78236	-1073.04388	-980.19888
12	H	-4.0690	26.00733	291.61876	0.15477	291.77354	317.78087
13	C	3.8960	92.85033	-1110.20619	36.77347	-1073.43272	-980.58238
14	H	-4.0720	26.00633	291.83377	0.15488	291.98865	317.99498
15	C	3.8980	92.82933	-1110.77611	36.80624	-1073.96987	-981.14054
16	H	-4.0720	26.00633	291.83377	0.15508	291.98884	317.99518
17	C	3.8990	92.82267	-1111.06107	36.81447	-1074.24660	-981.42393
18	H	-4.0707	26.00667	291.73821	0.15446	291.89267	317.89934
19	C	3.8973	92.83600	-1110.58614	36.79236	-1073.79377	-980.95777
20	C	3.8957	92.85400	-1110.11120	36.76639	-1073.34482	-980.49082
21	H	-4.0687	26.00667	291.59487	0.15420	291.74907	317.75574
13C Average		3.8968	92.83960	-1110.44366	36.79045	-1073.65320	-980.81360
1H Average		-4.0705	26.00660	291.72865	0.15455	291.88320	317.88980

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3NiCp2-STO-PBE-Van-Wullen

Temperature: 298

Spin: 1

atensor 1 Ni

91.492 0.000 0.011
0.000 91.492 0.006
0.011 0.006 4.436
-26.459 0.000 -0.003
0.000 -26.459 -0.002
-0.003 -0.002 -2.693

atensor 2 H

-7.318 -2.614 -0.914
-2.614 -0.894 2.571
-0.914 2.571 -3.927
-0.082 -0.032 -0.045
-0.032 -0.004 0.126
-0.010 0.029 0.010

atensor 3 C

-0.832 -0.227 -0.894
-0.227 -0.275 2.514
-0.894 2.514 13.176
-0.223 -0.033 -0.041
-0.033 -0.142 0.114
-0.014 0.040 -0.011

atensor 4 H

0.030 0.227 -2.728
0.227 -8.242 -0.075
-2.728 -0.075 -3.927
0.007 0.003 -0.134
0.003 -0.093 -0.004
-0.031 -0.001 0.010

atensor 5 C

-0.195 0.020 -2.667
0.020 -0.912 -0.073
-2.667 -0.073 13.176
-0.130 0.003 -0.121
0.003 -0.235 -0.003
-0.042 -0.001 -0.011

atensor 6 H

-7.584 2.247 -0.772
2.247 -0.626 -2.617
-0.772 -2.618 -3.926
-0.085 0.027 -0.038
0.027 -0.001 -0.128
-0.009 -0.030 0.010

atensor 7 C

-0.854 0.195 -0.754
0.195 -0.250 -2.559
-0.754 -2.560 13.172
-0.226 0.028 -0.034
0.028 -0.139 -0.116
-0.012 -0.041 -0.011

atensor 8 H

-2.610 -3.862 2.251
-3.862 -5.597 -1.543
2.251 -1.543 -3.925
-0.025 -0.047 0.110
-0.047 -0.061 -0.076

0.025 -0.017 0.010

atensor 9 C
-0.423 -0.335 2.201
-0.335 -0.682 -1.509
2.201 -1.509 13.166
-0.164 -0.049 0.100
-0.049 -0.201 -0.069
0.035 -0.024 -0.011

atensor 10 H
-3.042 4.003 2.163
4.003 -5.166 1.664
2.163 1.664 -3.925
-0.030 0.049 0.106
0.049 -0.056 0.082
0.024 0.019 0.010

atensor 11 C
-0.462 0.347 2.115
0.347 -0.646 1.626
2.115 1.626 13.168
-0.169 0.051 0.096
0.051 -0.196 0.074
0.034 0.026 -0.011

atensor 12 H
-7.581 2.247 0.772
2.247 -0.626 2.618
0.772 2.618 -3.924
-0.085 0.027 0.038
0.027 -0.001 0.128
0.009 0.030 0.010

atensor 13 C
-0.853 0.195 0.755
0.195 -0.251 2.557
0.755 2.557 13.167
-0.226 0.028 0.034
0.028 -0.138 0.116
0.012 0.041 -0.011

atensor 14 H
-2.613 -3.863 -2.251
-3.863 -5.600 1.543
-2.251 1.543 -3.927
-0.025 -0.047 -0.110
-0.047 -0.061 0.076
-0.025 0.017 0.010

atensor 15 C
-0.424 -0.335 -2.199
-0.335 -0.683 1.506
-2.199 1.507 13.177
-0.164 -0.049 -0.100
-0.049 -0.201 0.069
-0.035 0.024 -0.011

atensor 16 H
-3.045 4.004 -2.162
4.004 -5.168 -1.664
-2.162 -1.664 -3.927
-0.030 0.049 -0.106
0.049 -0.056 -0.082
-0.024 -0.019 0.010

atensor 17 C

-0.462 0.347 -2.113
0.347 -0.645 -1.627
-2.113 -1.627 13.180
-0.169 0.050 -0.096
0.050 -0.196 -0.074
-0.034 -0.026 -0.011

atensor 18 H
-7.317 -2.615 0.914
-2.615 -0.893 -2.571
0.914 -2.571 -3.926
-0.082 -0.032 0.045
-0.032 -0.004 -0.126
0.010 -0.029 0.010

atensor 19 C
-0.831 -0.227 0.894
-0.227 -0.274 -2.514
0.894 -2.514 13.173
-0.223 -0.033 0.041
-0.033 -0.142 -0.114
0.014 -0.040 -0.011

atensor 20 C
-0.192 0.020 2.667
0.020 -0.910 0.072
2.667 0.072 13.165
-0.130 0.003 0.121
0.003 -0.235 0.003
0.042 0.001 -0.011

atensor 21 H
0.031 0.227 2.728
0.227 -8.237 0.074
2.728 0.074 -3.924
0.007 0.003 0.134
0.003 -0.093 0.004
0.031 0.001 0.010

orbtensor 1 Ni
-7767.637 0.084 -0.155
0.084 -7767.606 -0.401
-0.155 -0.401 -641.847
2275.747 0.000 0.004
0.000 2275.746 0.001
0.004 0.001 2268.030

orbtensor 2 H
-0.428 3.596 0.742
3.596 -9.265 -2.088
0.742 -2.088 -0.559
26.153 -4.237 -1.205
-4.237 36.563 3.389
-1.205 3.389 25.554

orbtensor 3 C
-146.772 21.911 9.274
21.911 -200.592 -26.082
9.274 -26.082 -57.730
223.644 -5.761 -4.957
-5.761 237.799 13.942
-4.957 13.942 222.147

orbtensor 4 H
-10.535 -0.312 2.215
-0.312 0.842 0.061
2.215 0.061 -0.559

38.060	0.368	-3.595
0.368	24.657	-0.099
-3.595	-0.099	25.554

orbtensor 5 C

-208.335	-1.902	27.667
-1.902	-139.029	0.756
27.667	0.756	-57.727
239.836	0.500	-14.790
0.500	221.611	-0.406
-14.790	-0.406	222.146

orbtensor 6 H

-0.061	-3.091	0.626
-3.091	-9.631	2.125
0.626	2.125	-0.559
25.720	3.641	-1.017
3.641	36.996	-3.449
-1.017	-3.449	25.554

orbtensor 7 C

-144.515	-18.834	7.827
-18.834	-202.823	26.539
7.827	26.539	-57.728
223.057	4.951	-4.185
4.951	238.390	-14.191
-4.185	-14.191	222.147

orbtensor 8 H

-6.900	5.313	-1.827
5.313	-2.791	1.253
-1.827	1.253	-0.558
33.779	-6.260	2.966
-6.260	28.937	-2.033
2.966	-2.033	25.554

orbtensor 9 C

-186.171	32.372	-22.823
32.372	-161.140	15.643
-22.823	15.643	-57.729
234.012	-8.511	12.204
-8.511	227.430	-8.365
12.204	-8.365	222.148

orbtensor 10 H

-6.306	-5.506	-1.756
-5.506	-3.385	-1.351
-1.756	-1.351	-0.558
33.079	6.487	2.851
6.487	29.637	2.193
2.851	2.193	25.554

orbtensor 11 C

-182.556	-33.543	-21.934
-33.543	-164.770	-16.878
-21.934	-16.878	-57.729
233.061	8.820	11.727
8.820	228.381	9.023
11.727	9.023	222.148

orbtensor 12 H

-0.061	-3.090	-0.627
-3.090	-9.630	-2.126
-0.627	-2.126	-0.559
25.721	3.641	1.017
3.641	36.996	3.451
1.017	3.451	25.555

orbtensor 13 C
-144.497 -18.825 -7.822
-18.825 -202.808 -26.568
-7.822 -26.568 -57.733
223.054 4.951 4.183
4.951 238.384 14.195
4.183 14.195 222.151

orbtensor 14 H
-6.901 5.313 1.829
5.313 -2.792 -1.254
1.829 -1.254 -0.559
33.779 -6.259 -2.968
-6.259 28.938 2.034
-2.968 2.034 25.554

orbtensor 15 C
-186.207 32.363 22.857
32.363 -161.163 -15.666
22.857 -15.666 -57.736
234.014 -8.510 -12.207
-8.510 227.431 8.365
-12.207 8.365 222.149

orbtensor 16 H
-6.307 -5.507 1.757
-5.507 -3.387 1.352
1.757 1.352 -0.559
33.079 6.487 -2.851
6.487 29.639 -2.193
-2.851 -2.193 25.554

orbtensor 17 C
-182.595 -33.540 21.960
-33.540 -164.803 16.882
21.960 16.882 -57.727
233.062 8.821 -11.728
8.821 228.386 -9.022
-11.728 -9.022 222.145

orbtensor 18 H
-0.428 3.596 -0.743
3.596 -9.264 2.088
-0.743 2.088 -0.559
26.153 -4.237 1.204
-4.237 36.564 -3.388
1.204 -3.388 25.554

orbtensor 19 C
-146.756 21.903 -9.265
21.903 -200.597 26.083
-9.265 26.083 -57.725
223.643 -5.762 4.954
-5.762 237.799 -13.942
4.954 -13.942 222.144

orbtensor 20 C
-208.302 -1.897 -27.667
-1.897 -138.992 -0.764
-27.667 -0.764 -57.728
239.831 0.499 14.791
0.499 221.606 0.405
14.791 0.405 222.147

orbtensor 21 H
-10.533 -0.312 -2.215

```

-0.312    0.842   -0.061
-2.215   -0.061   -0.559
38.059    0.368    3.595
0.368    24.657    0.098
3.595     0.098    25.554

```

```

gtensor (ppt)
-0.046    0.000    0.000
 0.000   -0.046    0.000
 0.000    0.000   -0.208
42.117   -0.001    0.006
-0.001   42.116    0.003
 0.006    0.003    1.051

```

```

zfstensor (cm-1)
-5.981030 -0.000134    0.001055
-0.000134 -5.980978    0.000857
 0.001055  0.000857   11.962008

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.9363	-3119.18900	35168.34912	712.65400	35881.00312	32761.81412
2	H	-4.0717	26.00600	291.74563	0.23397	291.97960	317.98560
3	C	3.8977	92.83200	-1110.43661	55.71261	-1054.72400	-961.89200
4	H	-4.0717	26.00633	291.74563	0.23384	291.97947	317.98581
5	C	3.8977	92.83400	-1110.43661	55.71241	-1054.72420	-961.89020
6	H	-4.0707	26.00633	291.67398	0.23386	291.90784	317.91417
7	C	3.8973	92.84267	-1110.34164	55.68998	-1054.65166	-961.80899
8	H	-4.0693	26.00700	291.57845	0.23320	291.81165	317.81865
9	C	3.8950	92.85000	-1109.67688	55.66778	-1054.00910	-961.15910
10	H	-4.0697	26.00700	291.60233	0.23387	291.83620	317.84320
11	C	3.8947	92.84500	-1109.58191	55.68221	-1053.89970	-961.05470
12	H	-4.0690	26.00733	291.55456	0.23449	291.78905	317.79638
13	C	3.8960	92.85033	-1109.96178	55.66842	-1054.29336	-961.44303
14	H	-4.0720	26.00633	291.76952	0.23439	292.00391	318.01024
15	C	3.8980	92.82933	-1110.53157	55.71657	-1054.81501	-961.98567
16	H	-4.0720	26.00633	291.76952	0.23436	292.00388	318.01022
17	C	3.8990	92.82267	-1110.81647	55.72825	-1055.08822	-962.26556
18	H	-4.0707	26.00667	291.67398	0.23378	291.90776	317.91443
19	C	3.8973	92.83600	-1110.34164	55.69585	-1054.64579	-961.80979
20	C	3.8957	92.85400	-1109.86681	55.65791	-1054.20890	-961.35490
21	H	-4.0687	26.00667	291.53068	0.23374	291.76441	317.77108
13C Average		3.8968	92.83960	-1110.19919	55.69320	-1054.50599	-961.66639
1H Average		-4.0705	26.00660	291.66443	0.23395	291.89838	317.90498

```

=====
3NiCp2-STO-B3LYP-No-ZFS
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
106.636 0.000 0.006
0.000 106.636 0.006
0.006 0.006 5.323
-40.789 0.001 -0.004
0.001 -40.788 -0.002
-0.004 -0.002 -2.922

```

```

atensor 2 H
-6.815 -2.529 -1.039

```

-2.529 -0.602 2.922
-1.039 2.922 -3.454
-0.128 -0.060 -0.073
-0.060 0.018 0.204
-0.010 0.028 0.011

atensor 3 C
0.828 -0.309 -0.963
-0.309 1.587 2.708
-0.963 2.708 13.169
-0.285 -0.033 -0.061
-0.033 -0.203 0.171
-0.008 0.024 -0.011

atensor 4 H
0.291 0.220 -3.100
0.220 -7.709 -0.085
-3.100 -0.085 -3.455
0.039 0.005 -0.216
0.005 -0.149 -0.006
-0.029 -0.001 0.011

atensor 5 C
1.697 0.027 -2.874
0.027 0.719 -0.079
-2.874 -0.079 13.170
-0.191 0.003 -0.182
0.003 -0.297 -0.005
-0.025 -0.001 -0.011

atensor 6 H
-7.072 2.173 -0.877
2.173 -0.343 -2.975
-0.877 -2.975 -3.454
-0.134 0.051 -0.061
0.051 0.024 -0.208
-0.008 -0.028 0.011

atensor 7 C
0.798 0.265 -0.813
0.265 1.620 -2.757
-0.813 -2.757 13.165
-0.289 0.029 -0.051
0.029 -0.200 -0.174
-0.007 -0.024 -0.011

atensor 8 H
-2.262 -3.735 2.559
-3.735 -5.151 -1.754
2.559 -1.754 -3.452
-0.021 -0.088 0.179
-0.088 -0.089 -0.122
0.024 -0.017 0.011

atensor 9 C
1.385 -0.456 2.371
-0.456 1.032 -1.625
2.371 -1.625 13.160
-0.225 -0.050 0.150
-0.050 -0.263 -0.103
0.021 -0.014 -0.011

atensor 10 H
-2.680 3.871 2.458
3.871 -4.734 1.891
2.459 1.892 -3.453
-0.031 0.091 0.172

0.091 -0.079 0.132
0.023 0.018 0.011

atensor 11 C
1.332 0.473 2.278
0.473 1.081 1.753
2.278 1.753 13.161
-0.231 0.051 0.144
0.051 -0.258 0.111
0.020 0.015 -0.011

atensor 12 H
-7.070 2.173 0.877
2.173 -0.343 2.976
0.878 2.976 -3.451
-0.134 0.051 0.061
0.051 0.024 0.208
0.008 0.028 0.011

atensor 13 C
0.799 0.266 0.813
0.266 1.620 2.755
0.813 2.755 13.161
-0.289 0.029 0.051
0.029 -0.200 0.174
0.007 0.024 -0.011

atensor 14 H
-2.265 -3.736 -2.558
-3.736 -5.154 1.753
-2.559 1.753 -3.454
-0.021 -0.088 -0.178
-0.088 -0.089 0.122
-0.024 0.017 0.011

atensor 15 C
1.384 -0.456 -2.370
-0.456 1.031 1.623
-2.370 1.623 13.170
-0.225 -0.049 -0.150
-0.049 -0.263 0.103
-0.021 0.014 -0.011

atensor 16 H
-2.683 3.872 -2.457
3.872 -4.736 -1.891
-2.458 -1.891 -3.455
-0.031 0.091 -0.171
0.091 -0.079 -0.132
-0.023 -0.018 0.011

atensor 17 C
1.332 0.473 -2.277
0.473 1.082 -1.753
-2.277 -1.753 13.172
-0.231 0.051 -0.144
0.051 -0.258 -0.111
-0.020 -0.015 -0.011

atensor 18 H
-6.814 -2.529 1.039
-2.529 -0.601 -2.922
1.039 -2.922 -3.454
-0.128 -0.060 0.072
-0.060 0.018 -0.204
0.010 -0.028 0.011

atensor 19 C
0.829 -0.309 0.963
-0.309 1.588 -2.709
0.963 -2.709 13.165
-0.285 -0.033 0.061
-0.033 -0.203 -0.171
0.008 -0.024 -0.011

atensor 20 C
1.699 0.027 2.873
0.027 0.721 0.078
2.873 0.078 13.158
-0.191 0.003 0.182
0.003 -0.297 0.005
0.025 0.001 -0.011

atensor 21 H
0.293 0.219 3.101
0.219 -7.704 0.085
3.101 0.085 -3.451
0.039 0.005 0.216
0.005 -0.149 0.006
0.029 0.001 0.011

orbtensor 1 Ni
-10666.224 0.143 -0.338
0.143-10666.193 -0.578
-0.338 -0.578 -434.897
2259.020 0.000 0.002
0.000 2259.020 0.000
0.002 0.000 2270.434

orbtensor 2 H
-1.027 4.821 0.607
4.821 -12.872 -1.708
0.607 -1.708 -0.200
28.273 -4.767 -0.737
-4.767 39.986 2.072
-0.737 2.072 25.494

orbtensor 3 C
-181.346 15.825 6.700
15.825 -220.214 -18.841
6.700 -18.841 -70.170
255.689 2.228 -1.406
2.228 250.214 3.952
-1.406 3.952 232.174

orbtensor 4 H
-14.575 -0.419 1.811
-0.419 0.676 0.050
1.811 0.050 -0.200
41.670 0.414 -2.198
0.414 26.589 -0.060
-2.198 -0.060 25.494

orbtensor 5 C
-225.804 -1.373 19.985
-1.373 -175.751 0.544
19.985 0.544 -70.166
249.428 -0.193 -4.192
-0.193 256.476 -0.113
-4.192 -0.113 232.173

orbtensor 6 H
-0.534 -4.143 0.512
-4.143 -13.364 1.738

0.512	1.738	-0.200
27.785	4.097	-0.622
4.097	40.474	-2.109
-0.622	-2.109	25.493

orbtensor 7 C

-179.704	-13.604	5.655
-13.604	-221.818	19.167
5.655	19.167	-70.167
255.915	-1.915	-1.188
-1.915	249.985	-4.022
-1.188	-4.022	232.174

orbtensor 8 H

-9.702	7.122	-1.494
7.122	-4.194	1.025
-1.494	1.025	-0.200
36.853	-7.044	1.814
-7.044	31.405	-1.243
1.814	-1.243	25.493

orbtensor 9 C

-209.790	23.382	-16.484
23.382	-191.710	11.297
-16.484	11.297	-70.168
251.675	3.292	3.460
3.292	254.221	-2.371
3.460	-2.371	232.174

orbtensor 10 H

-8.906	-7.381	-1.436
-7.381	-4.991	-1.105
-1.436	-1.105	-0.200
36.065	7.299	1.743
7.299	32.193	1.341
1.743	1.341	25.493

orbtensor 11 C

-207.181	-24.227	-15.842
-24.227	-194.338	-12.193
-15.842	-12.193	-70.167
252.043	-3.412	3.323
-3.412	253.853	2.559
3.323	2.559	232.173

orbtensor 12 H

-0.533	-4.143	-0.513
-4.143	-13.363	-1.740
-0.513	-1.740	-0.200
27.786	4.097	0.622
4.097	40.473	2.111
0.622	2.111	25.494

orbtensor 13 C

-179.687	-13.597	-5.646
-13.597	-221.805	-19.198
-5.646	-19.198	-70.171
255.913	-1.915	1.182
-1.915	249.982	4.026
1.182	4.026	232.175

orbtensor 14 H

-9.704	7.122	1.497
7.122	-4.195	-1.026
1.497	-1.026	-0.200
36.854	-7.043	-1.817
-7.043	31.406	1.245

```

-1.817    1.245    25.494

orbtensor 15 C
-209.823   23.373   16.521
23.373  -191.737  -11.322
16.521  -11.322  -70.173
251.678    3.292   -3.463
3.292  254.225    2.371
-3.463    2.371  232.173

orbtensor 16 H
-8.908   -7.381    1.437
-7.381   -4.992    1.106
1.437    1.106   -0.200
36.066    7.299   -1.744
7.299   32.194   -1.341
-1.744   -1.341   25.493

orbtensor 17 C
-207.219  -24.220   15.873
-24.220  -194.371   12.195
15.873   12.195  -70.166
252.048   -3.412   -3.327
-3.412  253.858   -2.555
-3.327   -2.555  232.172

orbtensor 18 H
-1.027    4.821   -0.607
4.821  -12.872    1.707
-0.607    1.707   -0.200
28.273   -4.767    0.736
-4.767   39.987   -2.072
0.736   -2.072   25.493

orbtensor 19 C
-181.330   15.817   -6.689
15.817  -220.214   18.843
-6.689   18.843  -70.167
255.688    2.228    1.400
2.228  250.214   -3.953
1.400   -3.953  232.173

orbtensor 20 C
-225.771   -1.370  -19.984
-1.370  -175.709   -0.554
-19.984   -0.554  -70.168
249.423   -0.194    4.192
-0.194  256.471    0.116
4.192    0.116  232.174

orbtensor 21 H
-14.573   -0.418   -1.812
-0.418    0.677   -0.050
-1.812   -0.050   -0.200
41.670    0.414    2.198
0.414   26.589    0.060
2.198    0.060   25.493

gtensor (ppt)
-0.081    0.000    0.000
0.000   -0.081    0.000
0.000    0.000   -0.224
77.079   -0.002    0.006
-0.002   77.079    0.005
0.006    0.005    1.014

averaging

```


13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.6987	-4992.94667	36196.73608	423.63144	36620.36752	31627.42085
2	H	-3.6567	26.55133	265.07246	0.19124	265.26370	291.81503
3	C	5.0283	88.78233	-1449.30134	28.97958	-1420.32176	-1331.53943
4	H	-3.6573	26.55133	265.12079	0.19174	265.31253	291.86386
5	C	5.0290	88.78533	-1449.49349	28.98330	-1420.51019	-1331.72486
6	H	-3.6560	26.55133	265.02413	0.19156	265.21570	291.76703
7	C	5.0277	88.79500	-1449.10919	28.97038	-1420.13881	-1331.34381
8	H	-3.6547	26.55167	264.92748	0.19122	265.11870	291.67037
9	C	5.0260	88.80067	-1448.62881	28.95594	-1419.67287	-1330.87220
10	H	-3.6553	26.55133	264.97581	0.19086	265.16667	291.71800
11	C	5.0247	88.79433	-1448.24451	28.96287	-1419.28163	-1330.48730
12	H	-3.6543	26.55233	264.90332	0.19177	265.09509	291.64742
13	C	5.0267	88.80233	-1448.82096	28.95607	-1419.86489	-1331.06256
14	H	-3.6573	26.55167	265.12079	0.19214	265.31293	291.86460
15	C	5.0287	88.78100	-1449.39741	28.98327	-1420.41415	-1331.63315
16	H	-3.6577	26.55100	265.14495	0.19234	265.33729	291.88829
17	C	5.0287	88.77400	-1449.39741	28.99217	-1420.40524	-1331.63124
18	H	-3.6560	26.55133	265.02413	0.19105	265.21518	291.76652
19	C	5.0277	88.78800	-1449.10919	28.96920	-1420.13999	-1331.35199
20	C	5.0263	88.80667	-1448.72488	28.94661	-1419.77828	-1330.97161
21	H	-3.6537	26.55200	264.85499	0.19111	265.04610	291.59810
	ring 1H	-3.6559	26.55153	265.01688	0.19150	265.20839	291.75992
	ring 13C	5.0274	88.79097	-1449.02272	28.96994	-1420.05278	-1331.26181

3NiCp2-STO-B3LYP-ORCA

Temperature: 298

Spin: 1

atensor 1 Ni

106.636 0.000 0.006
 0.000 106.636 0.006
 0.006 0.006 5.323
 -40.789 0.001 -0.004
 0.001 -40.788 -0.002
 -0.004 -0.002 -2.922

atensor 2 H

-6.815 -2.529 -1.039
 -2.529 -0.602 2.922
 -1.039 2.922 -3.454
 -0.128 -0.060 -0.073
 -0.060 0.018 0.204
 -0.010 0.028 0.011

atensor 3 C

0.828 -0.309 -0.963
 -0.309 1.587 2.708
 -0.963 2.708 13.169
 -0.285 -0.033 -0.061
 -0.033 -0.203 0.171
 -0.008 0.024 -0.011

atensor 4 H

0.291 0.220 -3.100
 0.220 -7.709 -0.085
 -3.100 -0.085 -3.455
 0.039 0.005 -0.216
 0.005 -0.149 -0.006

-0.029 -0.001 0.011

atensor 5 C
1.697 0.027 -2.874
0.027 0.719 -0.079
-2.874 -0.079 13.170
-0.191 0.003 -0.182
0.003 -0.297 -0.005
-0.025 -0.001 -0.011

atensor 6 H
-7.072 2.173 -0.877
2.173 -0.343 -2.975
-0.877 -2.975 -3.454
-0.134 0.051 -0.061
0.051 0.024 -0.208
-0.008 -0.028 0.011

atensor 7 C
0.798 0.265 -0.813
0.265 1.620 -2.757
-0.813 -2.757 13.165
-0.289 0.029 -0.051
0.029 -0.200 -0.174
-0.007 -0.024 -0.011

atensor 8 H
-2.262 -3.735 2.559
-3.735 -5.151 -1.754
2.559 -1.754 -3.452
-0.021 -0.088 0.179
-0.088 -0.089 -0.122
0.024 -0.017 0.011

atensor 9 C
1.385 -0.456 2.371
-0.456 1.032 -1.625
2.371 -1.625 13.160
-0.225 -0.050 0.150
-0.050 -0.263 -0.103
0.021 -0.014 -0.011

atensor 10 H
-2.680 3.871 2.458
3.871 -4.734 1.891
2.459 1.892 -3.453
-0.031 0.091 0.172
0.091 -0.079 0.132
0.023 0.018 0.011

atensor 11 C
1.332 0.473 2.278
0.473 1.081 1.753
2.278 1.753 13.161
-0.231 0.051 0.144
0.051 -0.258 0.111
0.020 0.015 -0.011

atensor 12 H
-7.070 2.173 0.877
2.173 -0.343 2.976
0.878 2.976 -3.451
-0.134 0.051 0.061
0.051 0.024 0.208
0.008 0.028 0.011

atensor 13 C

0.799 0.266 0.813
0.266 1.620 2.755
0.813 2.755 13.161
-0.289 0.029 0.051
0.029 -0.200 0.174
0.007 0.024 -0.011

atensor 14 H
-2.265 -3.736 -2.558
-3.736 -5.154 1.753
-2.559 1.753 -3.454
-0.021 -0.088 -0.178
-0.088 -0.089 0.122
-0.024 0.017 0.011

atensor 15 C
1.384 -0.456 -2.370
-0.456 1.031 1.623
-2.370 1.623 13.170
-0.225 -0.049 -0.150
-0.049 -0.263 0.103
-0.021 0.014 -0.011

atensor 16 H
-2.683 3.872 -2.457
3.872 -4.736 -1.891
-2.458 -1.891 -3.455
-0.031 0.091 -0.171
0.091 -0.079 -0.132
-0.023 -0.018 0.011

atensor 17 C
1.332 0.473 -2.277
0.473 1.082 -1.753
-2.277 -1.753 13.172
-0.231 0.051 -0.144
0.051 -0.258 -0.111
-0.020 -0.015 -0.011

atensor 18 H
-6.814 -2.529 1.039
-2.529 -0.601 -2.922
1.039 -2.922 -3.454
-0.128 -0.060 0.072
-0.060 0.018 -0.204
0.010 -0.028 0.011

atensor 19 C
0.829 -0.309 0.963
-0.309 1.588 -2.709
0.963 -2.709 13.165
-0.285 -0.033 0.061
-0.033 -0.203 -0.171
0.008 -0.024 -0.011

atensor 20 C
1.699 0.027 2.873
0.027 0.721 0.078
2.873 0.078 13.158
-0.191 0.003 0.182
0.003 -0.297 0.005
0.025 0.001 -0.011

atensor 21 H
0.293 0.219 3.101
0.219 -7.704 0.085
3.101 0.085 -3.451

0.039 0.005 0.216
0.005 -0.149 0.006
0.029 0.001 0.011

orbtensor 1 Ni
-10666.224 0.143 -0.338
0.143-10666.193 -0.578
-0.338 -0.578 -434.897
2259.020 0.000 0.002
0.000 2259.020 0.000
0.002 0.000 2270.434

orbtensor 2 H
-1.027 4.821 0.607
4.821 -12.872 -1.708
0.607 -1.708 -0.200
28.273 -4.767 -0.737
-4.767 39.986 2.072
-0.737 2.072 25.494

orbtensor 3 C
-181.346 15.825 6.700
15.825 -220.214 -18.841
6.700 -18.841 -70.170
255.689 2.228 -1.406
2.228 250.214 3.952
-1.406 3.952 232.174

orbtensor 4 H
-14.575 -0.419 1.811
-0.419 0.676 0.050
1.811 0.050 -0.200
41.670 0.414 -2.198
0.414 26.589 -0.060
-2.198 -0.060 25.494

orbtensor 5 C
-225.804 -1.373 19.985
-1.373 -175.751 0.544
19.985 0.544 -70.166
249.428 -0.193 -4.192
-0.193 256.476 -0.113
-4.192 -0.113 232.173

orbtensor 6 H
-0.534 -4.143 0.512
-4.143 -13.364 1.738
0.512 1.738 -0.200
27.785 4.097 -0.622
4.097 40.474 -2.109
-0.622 -2.109 25.493

orbtensor 7 C
-179.704 -13.604 5.655
-13.604 -221.818 19.167
5.655 19.167 -70.167
255.915 -1.915 -1.188
-1.915 249.985 -4.022
-1.188 -4.022 232.174

orbtensor 8 H
-9.702 7.122 -1.494
7.122 -4.194 1.025
-1.494 1.025 -0.200
36.853 -7.044 1.814
-7.044 31.405 -1.243
1.814 -1.243 25.493

orbtensor 9 C
-209.790 23.382 -16.484
23.382 -191.710 11.297
-16.484 11.297 -70.168
251.675 3.292 3.460
3.292 254.221 -2.371
3.460 -2.371 232.174

orbtensor 10 H
-8.906 -7.381 -1.436
-7.381 -4.991 -1.105
-1.436 -1.105 -0.200
36.065 7.299 1.743
7.299 32.193 1.341
1.743 1.341 25.493

orbtensor 11 C
-207.181 -24.227 -15.842
-24.227 -194.338 -12.193
-15.842 -12.193 -70.167
252.043 -3.412 3.323
-3.412 253.853 2.559
3.323 2.559 232.173

orbtensor 12 H
-0.533 -4.143 -0.513
-4.143 -13.363 -1.740
-0.513 -1.740 -0.200
27.786 4.097 0.622
4.097 40.473 2.111
0.622 2.111 25.494

orbtensor 13 C
-179.687 -13.597 -5.646
-13.597 -221.805 -19.198
-5.646 -19.198 -70.171
255.913 -1.915 1.182
-1.915 249.982 4.026
1.182 4.026 232.175

orbtensor 14 H
-9.704 7.122 1.497
7.122 -4.195 -1.026
1.497 -1.026 -0.200
36.854 -7.043 -1.817
-7.043 31.406 1.245
-1.817 1.245 25.494

orbtensor 15 C
-209.823 23.373 16.521
23.373 -191.737 -11.322
16.521 -11.322 -70.173
251.678 3.292 -3.463
3.292 254.225 2.371
-3.463 2.371 232.173

orbtensor 16 H
-8.908 -7.381 1.437
-7.381 -4.992 1.106
1.437 1.106 -0.200
36.066 7.299 -1.744
7.299 32.194 -1.341
-1.744 -1.341 25.493

orbtensor 17 C
-207.219 -24.220 15.873

```

-24.220  -194.371  12.195
15.873   12.195  -70.166
252.048   -3.412  -3.327
-3.412   253.858  -2.555
-3.327   -2.555  232.172

```

```

orbtensor 18 H
-1.027   4.821  -0.607
4.821  -12.872   1.707
-0.607   1.707  -0.200
28.273  -4.767   0.736
-4.767   39.987  -2.072
0.736   -2.072  25.493

```

```

orbtensor 19 C
-181.330  15.817  -6.689
15.817 -220.214  18.843
-6.689  18.843  -70.167
255.688   2.228   1.400
2.228  250.214  -3.953
1.400  -3.953  232.173

```

```

orbtensor 20 C
-225.771  -1.370  -19.984
-1.370 -175.709  -0.554
-19.984  -0.554  -70.168
249.423  -0.194   4.192
-0.194  256.471   0.116
4.192   0.116  232.174

```

```

orbtensor 21 H
-14.573  -0.418  -1.812
-0.418   0.677  -0.050
-1.812  -0.050  -0.200
41.670   0.414   2.198
0.414   26.589   0.060
2.198   0.060  25.493

```

```

gtensor (ppt)
-0.081   0.000   0.000
0.000  -0.081   0.000
0.000   0.000  -0.224
77.079  -0.002   0.006
-0.002  77.079   0.005
0.006   0.005   1.014

```

```

zfstensor (cm-1)
42.93365   0.00028   0.00090
0.00028  42.93604   0.00011
0.00090   0.00011  53.57423

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.6987	-4992.94667	36199.04925	713.12495	36912.17420	31919.22754
2	H	-3.6567	26.55133	265.08915	0.32243	265.41158	291.96291
3	C	5.0283	88.78233	-1449.39767	48.78372	-1400.61395	-1311.83162
4	H	-3.6573	26.55133	265.13748	0.32153	265.45901	292.01034
5	C	5.0290	88.78533	-1449.58983	48.78678	-1400.80305	-1312.01772
6	H	-3.6560	26.55133	265.04082	0.32248	265.36330	291.91463
7	C	5.0277	88.79500	-1449.20551	48.76627	-1400.43924	-1311.64424
8	H	-3.6547	26.55167	264.94416	0.32205	265.26621	291.81787

9	C	5.0260	88.80067	-1448.72510	48.74468	-1399.98041	-1311.17975
10	H	-3.6553	26.55133	264.99249	0.32184	265.31433	291.86566
11	C	5.0247	88.79433	-1448.34077	48.75761	-1399.58316	-1310.78883
12	H	-3.6543	26.55233	264.91999	0.32379	265.24378	291.79611
13	C	5.0267	88.80233	-1448.91726	48.74565	-1400.17161	-1311.36927
14	H	-3.6573	26.55167	265.13748	0.32287	265.46034	292.01201
15	C	5.0287	88.78100	-1449.49375	48.78800	-1400.70576	-1311.92476
16	H	-3.6577	26.55100	265.16164	0.32294	265.48458	292.03558
17	C	5.0287	88.77400	-1449.49375	48.80180	-1400.69196	-1311.91796
18	H	-3.6560	26.55133	265.04082	0.32198	265.36280	291.91413
19	C	5.0277	88.78800	-1449.20551	48.76576	-1400.43975	-1311.65175
20	C	5.0263	88.80667	-1448.82118	48.72985	-1400.09133	-1311.28466
21	H	-3.6537	26.55200	264.87166	0.32179	265.19345	291.74545
13C Average		5.0274	88.79097	-1449.11903	48.76701	-1400.35202	-1311.56105
1H Average		-3.6559	26.55153	265.03357	0.32237	265.35594	291.90747

=====

3NiCp2-STO-BHLYP-ORCA

Temperature: 298

Spin: 1

atensor 1 Ni

134.673 0.000 0.001
0.000 134.674 0.007
0.001 0.007 15.675
-74.669 0.001 -0.005
0.001 -74.669 -0.004
-0.004 -0.004 -1.121

atensor 2 H

-5.983 -2.322 -1.200
-2.322 -0.276 3.375
-1.200 3.375 -2.648
-0.239 -0.129 -0.140
-0.129 0.077 0.392
-0.005 0.013 0.006

atensor 3 C

2.619 -0.396 -1.018
-0.396 3.591 2.864
-1.019 2.864 11.843
-0.407 -0.043 -0.109
-0.043 -0.302 0.305
0.000 0.000 -0.006

atensor 4 H

0.544 0.202 -3.581
0.202 -6.803 -0.098
-3.581 -0.098 -2.649
0.123 0.011 -0.416
0.011 -0.284 -0.011
-0.014 0.000 0.006

atensor 5 C

3.731 0.034 -3.039
0.034 2.479 -0.083
-3.039 -0.083 11.844
-0.287 0.004 -0.324
0.004 -0.423 -0.009
0.000 0.000 -0.006

atensor 6 H

-6.219 1.996 -1.013
1.996 -0.038 -3.436
-1.013 -3.436 -2.648
-0.252 0.111 -0.118

0.111 0.090 -0.400
-0.004 -0.014 0.006

atensor 7 C
2.579 0.340 -0.860
0.340 3.632 -2.916
-0.860 -2.916 11.840
-0.412 0.037 -0.092
0.037 -0.297 -0.311
0.000 0.000 -0.006

atensor 8 H
-1.801 -3.431 2.955
-3.431 -4.454 -2.026
2.955 -2.026 -2.646
-0.007 -0.190 0.344
-0.190 -0.154 -0.236
0.012 -0.008 0.006

atensor 9 C
3.331 -0.585 2.508
-0.585 2.879 -1.719
2.508 -1.719 11.835
-0.330 -0.064 0.267
-0.064 -0.379 -0.183
0.000 0.000 -0.006

atensor 10 H
-2.184 3.556 2.839
3.556 -4.071 2.184
2.839 2.185 -2.646
-0.029 0.197 0.330
0.197 -0.133 0.254
0.011 0.009 0.006

atensor 11 C
3.265 0.606 2.409
0.606 2.943 1.854
2.409 1.854 11.837
-0.337 0.066 0.257
0.066 -0.372 0.198
0.000 0.000 -0.006

atensor 12 H
-6.217 1.996 1.013
1.996 -0.038 3.437
1.013 3.437 -2.645
-0.252 0.111 0.118
0.111 0.090 0.400
0.004 0.014 0.006

atensor 13 C
2.579 0.340 0.860
0.340 3.632 2.915
0.860 2.915 11.836
-0.412 0.037 0.092
0.037 -0.297 0.311
0.000 0.000 -0.006

atensor 14 H
-1.803 -3.431 -2.955
-3.431 -4.457 2.025
-2.955 2.025 -2.647
-0.007 -0.190 -0.344
-0.190 -0.154 0.235
-0.012 0.008 0.006

atensor 15 C
3.331 -0.584 -2.507
-0.584 2.879 1.717
-2.507 1.717 11.845
-0.330 -0.064 -0.267
-0.064 -0.379 0.183
0.000 0.000 -0.006

atensor 16 H
-2.189 3.554 -2.838
3.554 -4.073 -2.184
-2.838 -2.184 -2.648
-0.029 0.197 -0.330
0.197 -0.133 -0.254
-0.011 -0.009 0.006

atensor 17 C
3.259 0.604 -2.409
0.604 2.939 -1.854
-2.409 -1.854 11.842
-0.337 0.066 -0.257
0.066 -0.372 -0.198
0.000 0.000 -0.006

atensor 18 H
-5.981 -2.322 1.199
-2.322 -0.275 -3.375
1.200 -3.375 -2.647
-0.239 -0.129 0.140
-0.129 0.077 -0.393
0.005 -0.013 0.006

atensor 19 C
2.618 -0.396 1.018
-0.396 3.591 -2.865
1.018 -2.865 11.839
-0.408 -0.043 0.109
-0.043 -0.302 -0.305
0.000 0.000 -0.006

atensor 20 C
3.732 0.034 3.039
0.034 2.480 0.082
3.039 0.082 11.833
-0.286 0.004 0.324
0.004 -0.423 0.009
0.000 0.000 -0.006

atensor 21 H
0.546 0.201 3.581
0.201 -6.799 0.098
3.582 0.098 -2.646
0.123 0.011 0.417
0.011 -0.284 0.011
0.014 0.000 0.006

orbtensor 1 Ni
-18958.147 0.290 -0.866
0.290-18958.068 -1.085
-0.866 -1.085 -220.649
2258.656 0.000 0.001
0.000 2258.656 -0.001
0.001 -0.001 2270.500

orbtensor 2 H
1.404 6.255 1.397
6.255 -13.964 -3.929

1.397	-3.929	-0.491
28.570	-4.657	-0.728
-4.657	40.014	2.048
-0.728	2.048	25.570

orbtensor 3 C

-169.201	17.197	9.289
17.197	-211.441	-26.123
9.289	-26.123	-63.009
256.792	3.044	-1.378
3.044	249.311	3.871
-1.378	3.871	231.507

orbtensor 4 H

-16.173	-0.543	4.167
-0.543	3.614	0.114
4.167	0.114	-0.490
41.659	0.405	-2.172
0.405	26.926	-0.060
-2.172	-0.060	25.570

orbtensor 5 C

-217.513	-1.493	27.711
-1.493	-163.120	0.756
27.711	0.756	-63.004
248.237	-0.264	-4.107
-0.264	257.867	-0.111
-4.107	-0.111	231.506

orbtensor 6 H

2.045	-5.376	1.179
-5.376	-14.602	3.999
1.179	3.999	-0.490
28.094	4.003	-0.615
4.003	40.490	-2.084
-0.615	-2.084	25.569

orbtensor 7 C

-167.416	-14.785	7.841
-14.785	-213.185	26.581
7.841	26.581	-63.004
257.101	-2.616	-1.164
-2.616	248.999	-3.940
-1.164	-3.940	231.507

orbtensor 8 H

-9.853	9.242	-3.439
9.242	-2.705	2.358
-3.439	2.358	-0.490
36.953	-6.881	1.792
-6.881	31.630	-1.229
1.792	-1.229	25.569

orbtensor 9 C

-200.118	25.413	-22.860
25.413	-180.467	15.667
-22.860	15.667	-63.007
251.309	4.498	3.389
4.498	254.787	-2.323
3.389	-2.323	231.507

orbtensor 10 H

-8.819	-9.578	-3.305
-9.578	-3.739	-2.542
-3.305	-2.542	-0.490
36.183	7.131	1.723
7.131	32.400	1.325

```

1.723      1.325      25.570

orbtensor 11 C
-197.282  -26.331  -21.968
-26.331  -183.323  -16.906
-21.968  -16.906  -63.007
251.812   -4.662   3.255
-4.662  254.285   2.507
3.255    2.507  231.507

orbtensor 12 H
2.045   -5.376   -1.180
-5.376  -14.601   -4.001
-1.180   -4.001   -0.491
28.094   4.003   0.614
4.003   40.489   2.087
0.614    2.087  25.570

orbtensor 13 C
-167.400  -14.780   -7.832
-14.780  -213.173  -26.613
-7.832  -26.613  -63.011
257.099   -2.616   1.157
-2.616  248.996   3.944
1.157    3.944  231.508

orbtensor 14 H
-9.852    9.240    3.441
9.240   -2.705   -2.358
3.441   -2.358   -0.490
36.953   -6.881   -1.795
-6.881   31.631    1.230
-1.795    1.230   25.570

orbtensor 15 C
-200.145   25.400   22.897
25.400  -180.492  -15.692
22.897  -15.692  -63.013
251.312    4.498   -3.393
4.498  254.791    2.323
-3.393    2.323  231.507

orbtensor 16 H
-8.819   -9.576    3.305
-9.576   -3.741    2.542
3.305    2.542   -0.490
36.184    7.131   -1.724
7.131   32.402   -1.326
-1.724   -1.326   25.570

orbtensor 17 C
-197.315  -26.323   21.997
-26.323  -183.352   16.908
21.997   16.908  -63.003
251.815   -4.660   -3.260
-4.660  254.289   -2.503
-3.260   -2.503  231.504

orbtensor 18 H
1.405    6.255   -1.396
6.255  -13.965    3.928
-1.396    3.928   -0.490
28.570   -4.657    0.727
-4.657   40.014   -2.048
0.727   -2.048   25.570

orbtensor 19 C

```

```

-169.186  17.192  -9.278
17.192 -211.443  26.127
-9.278  26.127 -63.005
256.791  3.044  1.372
3.044  249.310 -3.872
1.372  -3.872  231.506

```

```

orbtensor 20 C
-217.489  -1.489  -27.711
-1.489 -163.076  -0.766
-27.711  -0.766  -63.006
248.231  -0.265  4.106
-0.265  257.862  0.113
4.106  0.113  231.507

```

```

orbtensor 21 H
-16.173  -0.543  -4.169
-0.543  3.616  -0.114
-4.169  -0.114  -0.490
41.658  0.404  2.172
0.404  26.925  0.060
2.172  0.060  25.570

```

```

gtensor (ppt)
-0.111  0.000  0.000
0.000 -0.111  0.000
0.000  0.000 -0.249
161.193 -0.003  0.011
-0.003  161.192  0.010
0.011  0.010  0.378

```

```

zfstensor (cm-1)
43.08674  0.00037  -0.00024
0.00037  43.08625  0.00011
-0.00024  0.00011  48.50071

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.8543	-10449.68400	37317.06768	747.92308	38064.99076	27615.30676
2	H	-3.0210	27.03433	224.98720	0.83667	225.82387	252.85820
3	C	5.7793	97.98633	-1711.36148	53.21844	-1658.14304	-1560.15671
4	H	-3.0210	27.03533	224.98720	0.83644	225.82363	252.85897
5	C	5.7793	97.99100	-1711.36148	53.23269	-1658.12878	-1560.13778
6	H	-3.0203	27.03533	224.93755	0.83727	225.77481	252.81015
7	C	5.7787	98.00067	-1711.16406	53.20349	-1657.96058	-1559.95991
8	H	-3.0187	27.03467	224.81342	0.83588	225.64931	252.68398
9	C	5.7767	98.00367	-1710.57183	53.17156	-1657.40027	-1559.39660
10	H	-3.0190	27.03500	224.83825	0.83652	225.67477	252.70977
11	C	5.7767	97.99733	-1710.57183	53.18654	-1657.38529	-1559.38796
12	H	-3.0187	27.03533	224.81342	0.83798	225.65141	252.68674
13	C	5.7773	98.00633	-1710.76924	53.17258	-1657.59666	-1559.59033
14	H	-3.0207	27.03567	224.96237	0.83894	225.80131	252.83698
15	C	5.7800	97.98667	-1711.55889	53.23296	-1658.32593	-1560.33926
16	H	-3.0220	27.03533	225.06167	0.84148	225.90315	252.93848
17	C	5.7750	97.97933	-1710.07830	53.25434	-1656.82396	-1558.84463
18	H	-3.0197	27.03467	224.88790	0.83679	225.72469	252.75936
19	C	5.7773	97.99100	-1710.76924	53.20374	-1657.56550	-1559.57450
20	C	5.7767	98.00967	-1710.57183	53.15203	-1657.41980	-1559.41013
21	H	-3.0180	27.03533	224.76378	0.83421	225.59799	252.63332
13C Average		5.7777	97.99520	-1710.87782	53.20284	-1657.67498	-1559.67978

1H Average -3.0199 27.03510 224.90528 0.83722 225.74249 252.77759

=====

3NiCp2-STO-BHLYP-No-ZFS

Temperature: 298

Spin: 1

atensor 1 Ni

134.673 0.000 0.001
0.000 134.674 0.007
0.001 0.007 15.675
-74.669 0.001 -0.005
0.001 -74.669 -0.004
-0.004 -0.004 -1.121

atensor 2 H

-5.983 -2.322 -1.200
-2.322 -0.276 3.375
-1.200 3.375 -2.648
-0.239 -0.129 -0.140
-0.129 0.077 0.392
-0.005 0.013 0.006

atensor 3 C

2.619 -0.396 -1.018
-0.396 3.591 2.864
-1.019 2.864 11.843
-0.407 -0.043 -0.109
-0.043 -0.302 0.305
0.000 0.000 -0.006

atensor 4 H

0.544 0.202 -3.581
0.202 -6.803 -0.098
-3.581 -0.098 -2.649
0.123 0.011 -0.416
0.011 -0.284 -0.011
-0.014 0.000 0.006

atensor 5 C

3.731 0.034 -3.039
0.034 2.479 -0.083
-3.039 -0.083 11.844
-0.287 0.004 -0.324
0.004 -0.423 -0.009
0.000 0.000 -0.006

atensor 6 H

-6.219 1.996 -1.013
1.996 -0.038 -3.436
-1.013 -3.436 -2.648
-0.252 0.111 -0.118
0.111 0.090 -0.400
-0.004 -0.014 0.006

atensor 7 C

2.579 0.340 -0.860
0.340 3.632 -2.916
-0.860 -2.916 11.840
-0.412 0.037 -0.092
0.037 -0.297 -0.311
0.000 0.000 -0.006

atensor 8 H

-1.801 -3.431 2.955
-3.431 -4.454 -2.026
2.955 -2.026 -2.646

-0.007 -0.190 0.344
-0.190 -0.154 -0.236
0.012 -0.008 0.006

atensor 9 C
3.331 -0.585 2.508
-0.585 2.879 -1.719
2.508 -1.719 11.835
-0.330 -0.064 0.267
-0.064 -0.379 -0.183
0.000 0.000 -0.006

atensor 10 H
-2.184 3.556 2.839
3.556 -4.071 2.184
2.839 2.185 -2.646
-0.029 0.197 0.330
0.197 -0.133 0.254
0.011 0.009 0.006

atensor 11 C
3.265 0.606 2.409
0.606 2.943 1.854
2.409 1.854 11.837
-0.337 0.066 0.257
0.066 -0.372 0.198
0.000 0.000 -0.006

atensor 12 H
-6.217 1.996 1.013
1.996 -0.038 3.437
1.013 3.437 -2.645
-0.252 0.111 0.118
0.111 0.090 0.400
0.004 0.014 0.006

atensor 13 C
2.579 0.340 0.860
0.340 3.632 2.915
0.860 2.915 11.836
-0.412 0.037 0.092
0.037 -0.297 0.311
0.000 0.000 -0.006

atensor 14 H
-1.803 -3.431 -2.955
-3.431 -4.457 2.025
-2.955 2.025 -2.647
-0.007 -0.190 -0.344
-0.190 -0.154 0.235
-0.012 0.008 0.006

atensor 15 C
3.331 -0.584 -2.507
-0.584 2.879 1.717
-2.507 1.717 11.845
-0.330 -0.064 -0.267
-0.064 -0.379 0.183
0.000 0.000 -0.006

atensor 16 H
-2.189 3.554 -2.838
3.554 -4.073 -2.184
-2.838 -2.184 -2.648
-0.029 0.197 -0.330
0.197 -0.133 -0.254
-0.011 -0.009 0.006

atensor 17 C
3.259 0.604 -2.409
0.604 2.939 -1.854
-2.409 -1.854 11.842
-0.337 0.066 -0.257
0.066 -0.372 -0.198
0.000 0.000 -0.006

atensor 18 H
-5.981 -2.322 1.199
-2.322 -0.275 -3.375
1.200 -3.375 -2.647
-0.239 -0.129 0.140
-0.129 0.077 -0.393
0.005 -0.013 0.006

atensor 19 C
2.618 -0.396 1.018
-0.396 3.591 -2.865
1.018 -2.865 11.839
-0.408 -0.043 0.109
-0.043 -0.302 -0.305
0.000 0.000 -0.006

atensor 20 C
3.732 0.034 3.039
0.034 2.480 0.082
3.039 0.082 11.833
-0.286 0.004 0.324
0.004 -0.423 0.009
0.000 0.000 -0.006

atensor 21 H
0.546 0.201 3.581
0.201 -6.799 0.098
3.582 0.098 -2.646
0.123 0.011 0.417
0.011 -0.284 0.011
0.014 0.000 0.006

orbtensor 1 Ni
-18958.147 0.290 -0.866
0.290-18958.068 -1.085
-0.866 -1.085 -220.649
2258.656 0.000 0.001
0.000 2258.656 -0.001
0.001 -0.001 2270.500

orbtensor 2 H
1.404 6.255 1.397
6.255 -13.964 -3.929
1.397 -3.929 -0.491
28.570 -4.657 -0.728
-4.657 40.014 2.048
-0.728 2.048 25.570

orbtensor 3 C
-169.201 17.197 9.289
17.197 -211.441 -26.123
9.289 -26.123 -63.009
256.792 3.044 -1.378
3.044 249.311 3.871
-1.378 3.871 231.507

orbtensor 4 H
-16.173 -0.543 4.167

-0.543	3.614	0.114
4.167	0.114	-0.490
41.659	0.405	-2.172
0.405	26.926	-0.060
-2.172	-0.060	25.570
orbtensor 5 C		
-217.513	-1.493	27.711
-1.493	-163.120	0.756
27.711	0.756	-63.004
248.237	-0.264	-4.107
-0.264	257.867	-0.111
-4.107	-0.111	231.506
orbtensor 6 H		
2.045	-5.376	1.179
-5.376	-14.602	3.999
1.179	3.999	-0.490
28.094	4.003	-0.615
4.003	40.490	-2.084
-0.615	-2.084	25.569
orbtensor 7 C		
-167.416	-14.785	7.841
-14.785	-213.185	26.581
7.841	26.581	-63.004
257.101	-2.616	-1.164
-2.616	248.999	-3.940
-1.164	-3.940	231.507
orbtensor 8 H		
-9.853	9.242	-3.439
9.242	-2.705	2.358
-3.439	2.358	-0.490
36.953	-6.881	1.792
-6.881	31.630	-1.229
1.792	-1.229	25.569
orbtensor 9 C		
-200.118	25.413	-22.860
25.413	-180.467	15.667
-22.860	15.667	-63.007
251.309	4.498	3.389
4.498	254.787	-2.323
3.389	-2.323	231.507
orbtensor 10 H		
-8.819	-9.578	-3.305
-9.578	-3.739	-2.542
-3.305	-2.542	-0.490
36.183	7.131	1.723
7.131	32.400	1.325
1.723	1.325	25.570
orbtensor 11 C		
-197.282	-26.331	-21.968
-26.331	-183.323	-16.906
-21.968	-16.906	-63.007
251.812	-4.662	3.255
-4.662	254.285	2.507
3.255	2.507	231.507
orbtensor 12 H		
2.045	-5.376	-1.180
-5.376	-14.601	-4.001
-1.180	-4.001	-0.491
28.094	4.003	0.614

4.003	40.489	2.087
0.614	2.087	25.570

orbtensor 13 C

-167.400	-14.780	-7.832
-14.780	-213.173	-26.613
-7.832	-26.613	-63.011
257.099	-2.616	1.157
-2.616	248.996	3.944
1.157	3.944	231.508

orbtensor 14 H

-9.852	9.240	3.441
9.240	-2.705	-2.358
3.441	-2.358	-0.490
36.953	-6.881	-1.795
-6.881	31.631	1.230
-1.795	1.230	25.570

orbtensor 15 C

-200.145	25.400	22.897
25.400	-180.492	-15.692
22.897	-15.692	-63.013
251.312	4.498	-3.393
4.498	254.791	2.323
-3.393	2.323	231.507

orbtensor 16 H

-8.819	-9.576	3.305
-9.576	-3.741	2.542
3.305	2.542	-0.490
36.184	7.131	-1.724
7.131	32.402	-1.326
-1.724	-1.326	25.570

orbtensor 17 C

-197.315	-26.323	21.997
-26.323	-183.352	16.908
21.997	16.908	-63.003
251.815	-4.660	-3.260
-4.660	254.289	-2.503
-3.260	-2.503	231.504

orbtensor 18 H

1.405	6.255	-1.396
6.255	-13.965	3.928
-1.396	3.928	-0.490
28.570	-4.657	0.727
-4.657	40.014	-2.048
0.727	-2.048	25.570

orbtensor 19 C

-169.186	17.192	-9.278
17.192	-211.443	26.127
-9.278	26.127	-63.005
256.791	3.044	1.372
3.044	249.310	-3.872
1.372	-3.872	231.506

orbtensor 20 C

-217.489	-1.489	-27.711
-1.489	-163.076	-0.766
-27.711	-0.766	-63.006
248.231	-0.265	4.106
-0.265	257.862	0.113
4.106	0.113	231.507

```

orbtensor 21 H
-16.173  -0.543  -4.169
-0.543   3.616  -0.114
-4.169  -0.114  -0.490
41.658   0.404   2.172
0.404   26.925   0.060
2.172   0.060   25.570

```

```

gtensor (ppt)
-0.111   0.000   0.000
0.000  -0.111   0.000
0.000   0.000  -0.249
161.193  -0.003   0.011
-0.003  161.192   0.010
0.011   0.010   0.378

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	44.8543	-10449.68400	37310.22332	640.93845	37951.16177	27501.47777
2	H	-3.0210	27.03433	224.94593	0.71700	225.66293	252.69727
3	C	5.7793	97.98633	-1711.04759	45.60557	-1665.44202	-1567.45569
4	H	-3.0210	27.03533	224.94593	0.71673	225.66266	252.69800
5	C	5.7793	97.99100	-1711.04759	45.61827	-1665.42932	-1567.43832
6	H	-3.0203	27.03533	224.89629	0.71771	225.61400	252.64933
7	C	5.7787	98.00067	-1710.85022	45.59376	-1665.25646	-1567.25579
8	H	-3.0187	27.03467	224.77219	0.71644	225.48863	252.52330
9	C	5.7767	98.00367	-1710.25809	45.56602	-1664.69208	-1566.68841
10	H	-3.0190	27.03500	224.79701	0.71658	225.51359	252.54859
11	C	5.7767	97.99733	-1710.25809	45.57803	-1664.68006	-1566.68272
12	H	-3.0187	27.03533	224.77219	0.71796	225.49015	252.52549
13	C	5.7773	98.00633	-1710.45547	45.56607	-1664.88940	-1566.88306
14	H	-3.0207	27.03567	224.92111	0.71895	225.64006	252.67572
15	C	5.7800	97.98667	-1711.24497	45.61826	-1665.62671	-1567.64004
16	H	-3.0220	27.03533	225.02039	0.72112	225.74151	252.77685
17	C	5.7750	97.97933	-1709.76465	45.63710	-1664.12755	-1566.14822
18	H	-3.0197	27.03467	224.84665	0.71739	225.56405	252.59871
19	C	5.7773	97.99100	-1710.45547	45.59395	-1664.86152	-1566.87052
20	C	5.7767	98.00967	-1710.25809	45.54878	-1664.70931	-1566.69965
21	H	-3.0180	27.03533	224.72255	0.71472	225.43727	252.47260
13C Average		5.7777	97.99520	-1710.56402	45.59258	-1664.97144	-1566.97624
1H Average		-3.0199	27.03510	224.86403	0.71746	225.58149	252.61659

```

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3NiCp2-STO-PBE0-No-ZFS
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
122.260 0.000 0.005
0.000 122.260 0.006
0.005 0.006 17.302
-45.769 0.001 -0.004
0.001 -45.769 -0.003
-0.004 -0.003 -2.544

```

```

atensor 2 H
-6.721 -2.464 -1.066
-2.464 -0.665 2.999
-1.067 2.999 -3.334
-0.144 -0.069 -0.082

```

-0.069 0.026 0.231
-0.009 0.025 0.010

atensor 3 C
0.959 -0.328 -0.995
-0.328 1.765 2.798
-0.995 2.798 12.359
-0.302 -0.036 -0.068
-0.036 -0.214 0.192
-0.006 0.017 -0.010

atensor 4 H
0.205 0.214 -3.182
0.214 -7.591 -0.087
-3.182 -0.087 -3.335
0.051 0.006 -0.245
0.006 -0.169 -0.007
-0.026 -0.001 0.010

atensor 5 C
1.880 0.029 -2.969
0.029 0.843 -0.081
-2.969 -0.081 12.359
-0.201 0.003 -0.204
0.003 -0.315 -0.006
-0.018 -0.001 -0.010

atensor 6 H
-6.971 2.118 -0.900
2.118 -0.412 -3.054
-0.901 -3.054 -3.334
-0.151 0.060 -0.069
0.060 0.033 -0.236
-0.007 -0.025 0.010

atensor 7 C
0.927 0.282 -0.840
0.282 1.800 -2.849
-0.840 -2.849 12.356
-0.306 0.031 -0.058
0.031 -0.210 -0.196
-0.005 -0.018 -0.010

atensor 8 H
-2.283 -3.640 2.626
-3.640 -5.098 -1.800
2.626 -1.800 -3.332
-0.019 -0.103 0.203
-0.103 -0.099 -0.139
0.022 -0.015 0.010

atensor 9 C
1.550 -0.485 2.450
-0.485 1.175 -1.679
2.450 -1.679 12.350
-0.238 -0.053 0.168
-0.053 -0.279 -0.115
0.015 -0.010 -0.010

atensor 10 H
-2.690 3.773 2.523
3.773 -4.692 1.941
2.523 1.941 -3.332
-0.031 0.106 0.195
0.106 -0.087 0.150
0.021 0.016 0.010

atensor 11 C
1.495 0.502 2.354
0.502 1.228 1.811
2.354 1.811 12.353
-0.244 0.055 0.162
0.055 -0.273 0.124
0.015 0.011 -0.010

atensor 12 H
-6.968 2.117 0.901
2.117 -0.412 3.054
0.901 3.054 -3.331
-0.151 0.060 0.069
0.060 0.033 0.236
0.007 0.025 0.010

atensor 13 C
0.927 0.282 0.840
0.282 1.799 2.847
0.840 2.847 12.351
-0.306 0.031 0.058
0.031 -0.210 0.196
0.005 0.018 -0.010

atensor 14 H
-2.285 -3.641 -2.626
-3.641 -5.101 1.799
-2.626 1.800 -3.334
-0.019 -0.102 -0.203
-0.102 -0.099 0.139
-0.022 0.015 0.010

atensor 15 C
1.549 -0.484 -2.449
-0.484 1.174 1.677
-2.449 1.677 12.361
-0.238 -0.053 -0.168
-0.053 -0.279 0.115
-0.015 0.010 -0.010

atensor 16 H
-2.693 3.774 -2.522
3.774 -4.694 -1.941
-2.522 -1.941 -3.335
-0.031 0.106 -0.195
0.106 -0.087 -0.150
-0.021 -0.016 0.010

atensor 17 C
1.494 0.502 -2.353
0.502 1.228 -1.811
-2.353 -1.811 12.362
-0.243 0.055 -0.162
0.055 -0.273 -0.124
-0.015 -0.011 -0.010

atensor 18 H
-6.719 -2.464 1.066
-2.464 -0.664 -2.999
1.066 -2.999 -3.334
-0.144 -0.069 0.082
-0.069 0.026 -0.231
0.009 -0.025 0.010

atensor 19 C
0.960 -0.328 0.995
-0.328 1.766 -2.798

0.995 -2.799 12.356
-0.302 -0.036 0.068
-0.036 -0.214 -0.192
0.006 -0.017 -0.010

atensor 20 C
1.883 0.028 2.969
0.028 0.846 0.080
2.969 0.080 12.349
-0.201 0.003 0.204
0.003 -0.315 0.006
0.018 0.000 -0.010

atensor 21 H
0.207 0.214 3.183
0.214 -7.586 0.087
3.183 0.087 -3.331
0.051 0.006 0.246
0.006 -0.169 0.007
0.026 0.001 0.010

orbtensor 1 Ni
-11847.878 0.157 -0.449
0.157 -11847.827 -0.662
-0.449 -0.662 -383.621
2258.651 0.000 0.002
0.000 2258.651 -0.001
0.002 -0.001 2270.700

orbtensor 2 H
-0.535 5.101 0.750
5.101 -13.067 -2.110
0.750 -2.110 -0.262
27.938 -4.921 -0.778
-4.921 40.030 2.189
-0.778 2.189 25.203

orbtensor 3 C
-175.770 15.004 6.987
15.004 -212.618 -19.648
6.987 -19.648 -65.386
256.329 2.459 -1.435
2.459 250.284 4.033
-1.435 4.033 232.895

orbtensor 4 H
-14.869 -0.443 2.238
-0.443 1.267 0.062
2.238 0.062 -0.262
41.768 0.428 -2.321
0.428 26.200 -0.064
-2.321 -0.064 25.203

orbtensor 5 C
-217.917 -1.302 20.841
-1.302 -170.464 0.567
20.841 0.567 -65.382
249.417 -0.214 -4.279
-0.214 257.198 -0.116
-4.279 -0.116 232.894

orbtensor 6 H
-0.013 -4.384 0.633
-4.384 -13.587 2.147
0.633 2.147 -0.262
27.435 4.229 -0.657
4.229 40.533 -2.228

```

-0.657   -2.228   25.203

orbtensor 7 C
-174.212  -12.898    5.897
-12.898  -214.139   19.989
 5.897   19.989  -65.383
256.578   -2.114   -1.212
-2.114   250.032  -4.105
-1.212   -4.105  232.895

orbtensor 8 H
-9.714    7.536   -1.847
 7.536   -3.886    1.266
-1.847    1.266   -0.262
36.795   -7.271    1.916
-7.271   31.172   -1.313
 1.916   -1.313   25.203

orbtensor 9 C
-202.736  22.169  -17.191
 22.169 -185.594  11.781
-17.191  11.781  -65.384
251.898   3.634   3.531
 3.634  254.708  -2.420
 3.531  -2.420  232.895

orbtensor 10 H
-8.871   -7.810   -1.775
-7.810   -4.729   -1.365
-1.775   -1.365   -0.262
35.982    7.535    1.841
 7.535   31.985    1.416
 1.841    1.416   25.203

orbtensor 11 C
-200.262  -22.969  -16.521
-22.969 -188.087  -12.715
-16.521  -12.715  -65.384
252.304   -3.766    3.392
-3.766  254.303    2.612
 3.392    2.612  232.894

orbtensor 12 H
-0.013   -4.383   -0.634
-4.383  -13.587   -2.150
-0.634   -2.150   -0.262
27.435    4.229    0.657
 4.229   40.532    2.230
 0.657    2.230   25.204

orbtensor 13 C
-174.196  -12.892   -5.887
-12.892  -214.126  -20.020
-5.887  -20.020  -65.387
256.577   -2.114    1.206
-2.114   250.029    4.109
 1.206    4.109  232.896

orbtensor 14 H
-9.715    7.535    1.849
 7.535   -3.887   -1.267
 1.849   -1.267   -0.262
36.796   -7.270   -1.918
-7.270   31.172    1.314
-1.918    1.314   25.203

orbtensor 15 C

```

```
-202.768    22.158    17.227
22.158  -185.621   -11.805
17.227   -11.805   -65.390
251.901     3.635    -3.535
3.635   254.713     2.420
-3.535     2.420   232.895
```

```
orbtensor 16 H
-8.873    -7.809     1.776
-7.809    -4.730     1.366
1.776     1.366    -0.262
35.983     7.535    -1.842
7.535    31.986    -1.417
-1.842    -1.417    25.203
```

```
orbtensor 17 C
-200.301  -22.962    16.551
-22.962  -188.120    12.717
16.551   12.717   -65.382
252.309   -3.767    -3.396
-3.767   254.308    -2.608
-3.396   -2.608   232.893
```

```
orbtensor 18 H
-0.534     5.100    -0.750
5.100   -13.067     2.110
-0.750     2.110    -0.262
27.938   -4.921     0.777
-4.921   40.030    -2.188
0.777    -2.188    25.203
```

```
orbtensor 19 C
-175.756   14.996    -6.975
14.996  -212.624    19.650
-6.975   19.650   -65.384
256.328     2.460     1.429
2.460   250.284    -4.034
1.429   -4.034   232.894
```

```
orbtensor 20 C
-217.890   -1.297   -20.840
-1.297  -170.425   -0.578
-20.840   -0.578   -65.385
249.411   -0.215     4.279
-0.215   257.193     0.118
4.279     0.118   232.895
```

```
orbtensor 21 H
-14.867   -0.443   -2.239
-0.443    1.268   -0.061
-2.239   -0.061   -0.262
41.767    0.427    2.322
0.427   26.200    0.064
2.322    0.064   25.203
```

```
gtensor (ppt)
-0.089     0.000     0.000
0.000   -0.089     0.000
0.000     0.000   -0.231
89.311   -0.002     0.007
-0.002   89.311     0.005
0.007     0.005     0.841
```

```
averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21
```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.9133	-5763.77467	45456.64031	479.28062	45935.92093	40172.14626
2	H	-3.6093	26.43567	262.67148	0.29715	262.96863	289.40430
3	C	4.8523	95.24467	-1404.08526	31.07294	-1373.01232	-1277.76765
4	H	-3.6097	26.43567	262.69574	0.29733	262.99307	289.42873
5	C	4.8520	95.24867	-1403.98881	31.07714	-1372.91167	-1277.66301
6	H	-3.6083	26.43633	262.59870	0.29704	262.89575	289.33208
7	C	4.8523	95.25700	-1404.08526	31.06327	-1373.02199	-1277.76499
8	H	-3.6070	26.43600	262.50167	0.29670	262.79837	289.23437
9	C	4.8493	95.26233	-1403.21717	31.04787	-1372.16930	-1276.90697
10	H	-3.6073	26.43600	262.52593	0.29697	262.82289	289.25889
11	C	4.8497	95.25600	-1403.31363	31.05750	-1372.25613	-1277.00013
12	H	-3.6063	26.43633	262.45315	0.29703	262.75018	289.18651
13	C	4.8503	95.26433	-1403.50654	31.04693	-1372.45961	-1277.19528
14	H	-3.6093	26.43567	262.67148	0.29751	262.96899	289.40465
15	C	4.8523	95.24333	-1404.08526	31.08273	-1373.00253	-1277.75920
16	H	-3.6100	26.43567	262.72000	0.29796	263.01796	289.45362
17	C	4.8527	95.23567	-1404.18172	31.08733	-1373.09439	-1277.85872
18	H	-3.6083	26.43600	262.59870	0.29648	262.89518	289.33118
19	C	4.8520	95.24733	-1403.98881	31.06325	-1372.92556	-1277.67822
20	C	4.8507	95.26633	-1403.60299	31.03710	-1372.56589	-1277.29956
21	H	-3.6060	26.43633	262.42889	0.29656	262.72545	289.16179
13C Average		4.8514	95.25257	-1403.80554	31.06360	-1372.74194	-1277.48937
1H Average		-3.6082	26.43597	262.58657	0.29707	262.88365	289.31961

=====
 3NiCp2-STO-PBE0-ORCA
 Temperature: 298
 Spin: 1

atensor 1 Ni
 122.260 0.000 0.005
 0.000 122.260 0.006
 0.005 0.006 17.302
 -45.769 0.001 -0.004
 0.001 -45.769 -0.003
 -0.004 -0.003 -2.544

atensor 2 H
 -6.721 -2.464 -1.066
 -2.464 -0.665 2.999
 -1.067 2.999 -3.334
 -0.144 -0.069 -0.082
 -0.069 0.026 0.231
 -0.009 0.025 0.010

atensor 3 C
 0.959 -0.328 -0.995
 -0.328 1.765 2.798
 -0.995 2.798 12.359
 -0.302 -0.036 -0.068
 -0.036 -0.214 0.192
 -0.006 0.017 -0.010

atensor 4 H
 0.205 0.214 -3.182
 0.214 -7.591 -0.087
 -3.182 -0.087 -3.335
 0.051 0.006 -0.245
 0.006 -0.169 -0.007
 -0.026 -0.001 0.010

atensor 5 C

1.880 0.029 -2.969
0.029 0.843 -0.081
-2.969 -0.081 12.359
-0.201 0.003 -0.204
0.003 -0.315 -0.006
-0.018 -0.001 -0.010

atensor 6 H
-6.971 2.118 -0.900
2.118 -0.412 -3.054
-0.901 -3.054 -3.334
-0.151 0.060 -0.069
0.060 0.033 -0.236
-0.007 -0.025 0.010

atensor 7 C
0.927 0.282 -0.840
0.282 1.800 -2.849
-0.840 -2.849 12.356
-0.306 0.031 -0.058
0.031 -0.210 -0.196
-0.005 -0.018 -0.010

atensor 8 H
-2.283 -3.640 2.626
-3.640 -5.098 -1.800
2.626 -1.800 -3.332
-0.019 -0.103 0.203
-0.103 -0.099 -0.139
0.022 -0.015 0.010

atensor 9 C
1.550 -0.485 2.450
-0.485 1.175 -1.679
2.450 -1.679 12.350
-0.238 -0.053 0.168
-0.053 -0.279 -0.115
0.015 -0.010 -0.010

atensor 10 H
-2.690 3.773 2.523
3.773 -4.692 1.941
2.523 1.941 -3.332
-0.031 0.106 0.195
0.106 -0.087 0.150
0.021 0.016 0.010

atensor 11 C
1.495 0.502 2.354
0.502 1.228 1.811
2.354 1.811 12.353
-0.244 0.055 0.162
0.055 -0.273 0.124
0.015 0.011 -0.010

atensor 12 H
-6.968 2.117 0.901
2.117 -0.412 3.054
0.901 3.054 -3.331
-0.151 0.060 0.069
0.060 0.033 0.236
0.007 0.025 0.010

atensor 13 C
0.927 0.282 0.840
0.282 1.799 2.847
0.840 2.847 12.351

-0.306 0.031 0.058
0.031 -0.210 0.196
0.005 0.018 -0.010

atensor 14 H
-2.285 -3.641 -2.626
-3.641 -5.101 1.799
-2.626 1.800 -3.334
-0.019 -0.102 -0.203
-0.102 -0.099 0.139
-0.022 0.015 0.010

atensor 15 C
1.549 -0.484 -2.449
-0.484 1.174 1.677
-2.449 1.677 12.361
-0.238 -0.053 -0.168
-0.053 -0.279 0.115
-0.015 0.010 -0.010

atensor 16 H
-2.693 3.774 -2.522
3.774 -4.694 -1.941
-2.522 -1.941 -3.335
-0.031 0.106 -0.195
0.106 -0.087 -0.150
-0.021 -0.016 0.010

atensor 17 C
1.494 0.502 -2.353
0.502 1.228 -1.811
-2.353 -1.811 12.362
-0.243 0.055 -0.162
0.055 -0.273 -0.124
-0.015 -0.011 -0.010

atensor 18 H
-6.719 -2.464 1.066
-2.464 -0.664 -2.999
1.066 -2.999 -3.334
-0.144 -0.069 0.082
-0.069 0.026 -0.231
0.009 -0.025 0.010

atensor 19 C
0.960 -0.328 0.995
-0.328 1.766 -2.798
0.995 -2.799 12.356
-0.302 -0.036 0.068
-0.036 -0.214 -0.192
0.006 -0.017 -0.010

atensor 20 C
1.883 0.028 2.969
0.028 0.846 0.080
2.969 0.080 12.349
-0.201 0.003 0.204
0.003 -0.315 0.006
0.018 0.000 -0.010

atensor 21 H
0.207 0.214 3.183
0.214 -7.586 0.087
3.183 0.087 -3.331
0.051 0.006 0.246
0.006 -0.169 0.007
0.026 0.001 0.010

orbtensor 1 Ni
-11847.878 0.157 -0.449
0.157 -11847.827 -0.662
-0.449 -0.662 -383.621
2258.651 0.000 0.002
0.000 2258.651 -0.001
0.002 -0.001 2270.700

orbtensor 2 H
-0.535 5.101 0.750
5.101 -13.067 -2.110
0.750 -2.110 -0.262
27.938 -4.921 -0.778
-4.921 40.030 2.189
-0.778 2.189 25.203

orbtensor 3 C
-175.770 15.004 6.987
15.004 -212.618 -19.648
6.987 -19.648 -65.386
256.329 2.459 -1.435
2.459 250.284 4.033
-1.435 4.033 232.895

orbtensor 4 H
-14.869 -0.443 2.238
-0.443 1.267 0.062
2.238 0.062 -0.262
41.768 0.428 -2.321
0.428 26.200 -0.064
-2.321 -0.064 25.203

orbtensor 5 C
-217.917 -1.302 20.841
-1.302 -170.464 0.567
20.841 0.567 -65.382
249.417 -0.214 -4.279
-0.214 257.198 -0.116
-4.279 -0.116 232.894

orbtensor 6 H
-0.013 -4.384 0.633
-4.384 -13.587 2.147
0.633 2.147 -0.262
27.435 4.229 -0.657
4.229 40.533 -2.228
-0.657 -2.228 25.203

orbtensor 7 C
-174.212 -12.898 5.897
-12.898 -214.139 19.989
5.897 19.989 -65.383
256.578 -2.114 -1.212
-2.114 250.032 -4.105
-1.212 -4.105 232.895

orbtensor 8 H
-9.714 7.536 -1.847
7.536 -3.886 1.266
-1.847 1.266 -0.262
36.795 -7.271 1.916
-7.271 31.172 -1.313
1.916 -1.313 25.203

orbtensor 9 C
-202.736 22.169 -17.191

22.169	-185.594	11.781
-17.191	11.781	-65.384
251.898	3.634	3.531
3.634	254.708	-2.420
3.531	-2.420	232.895

orbtensor 10 H

-8.871	-7.810	-1.775
-7.810	-4.729	-1.365
-1.775	-1.365	-0.262
35.982	7.535	1.841
7.535	31.985	1.416
1.841	1.416	25.203

orbtensor 11 C

-200.262	-22.969	-16.521
-22.969	-188.087	-12.715
-16.521	-12.715	-65.384
252.304	-3.766	3.392
-3.766	254.303	2.612
3.392	2.612	232.894

orbtensor 12 H

-0.013	-4.383	-0.634
-4.383	-13.587	-2.150
-0.634	-2.150	-0.262
27.435	4.229	0.657
4.229	40.532	2.230
0.657	2.230	25.204

orbtensor 13 C

-174.196	-12.892	-5.887
-12.892	-214.126	-20.020
-5.887	-20.020	-65.387
256.577	-2.114	1.206
-2.114	250.029	4.109
1.206	4.109	232.896

orbtensor 14 H

-9.715	7.535	1.849
7.535	-3.887	-1.267
1.849	-1.267	-0.262
36.796	-7.270	-1.918
-7.270	31.172	1.314
-1.918	1.314	25.203

orbtensor 15 C

-202.768	22.158	17.227
22.158	-185.621	-11.805
17.227	-11.805	-65.390
251.901	3.635	-3.535
3.635	254.713	2.420
-3.535	2.420	232.895

orbtensor 16 H

-8.873	-7.809	1.776
-7.809	-4.730	1.366
1.776	1.366	-0.262
35.983	7.535	-1.842
7.535	31.986	-1.417
-1.842	-1.417	25.203

orbtensor 17 C

-200.301	-22.962	16.551
-22.962	-188.120	12.717
16.551	12.717	-65.382
252.309	-3.767	-3.396

-3.767 254.308 -2.608
 -3.396 -2.608 232.893

orbtensor 18 H
 -0.534 5.100 -0.750
 5.100 -13.067 2.110
 -0.750 2.110 -0.262
 27.938 -4.921 0.777
 -4.921 40.030 -2.188
 0.777 -2.188 25.203

orbtensor 19 C
 -175.756 14.996 -6.975
 14.996 -212.624 19.650
 -6.975 19.650 -65.384
 256.328 2.460 1.429
 2.460 250.284 -4.034
 1.429 -4.034 232.894

orbtensor 20 C
 -217.890 -1.297 -20.840
 -1.297 -170.425 -0.578
 -20.840 -0.578 -65.385
 249.411 -0.215 4.279
 -0.215 257.193 0.118
 4.279 0.118 232.895

orbtensor 21 H
 -14.867 -0.443 -2.239
 -0.443 1.268 -0.061
 -2.239 -0.061 -0.262
 41.767 0.427 2.322
 0.427 26.200 0.064
 2.322 0.064 25.203

gtensor (ppt)
 -0.089 0.000 0.000
 0.000 -0.089 0.000
 0.000 0.000 -0.231
 89.311 -0.002 0.007
 -0.002 89.311 0.005
 0.007 0.005 0.841

zfstensor (cm-1)
 47.402640 0.000723 0.000545
 0.000723 47.402293 -0.000003
 0.000545 -0.000003 49.021082

ss0tensor
 1.6224539723977717e20,-2.828079080878111e14,-2.1318161935629566e14
 -2.8280791030900844e14,1.6224553297192596e20,1.1734777445284097e12
 -2.1318161935629566e14,1.173475827010374e12,1.616123291897255e20

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.9133	-5763.77467	45458.33872	522.29121	45980.62993	40216.85527
2	H	-3.6093	26.43567	262.68154	0.32349	263.00504	289.44070
3	C	4.8523	95.24467	-1404.13413	33.86098	-1370.27315	-1275.02848
4	H	-3.6097	26.43567	262.70580	0.32385	263.02965	289.46532
5	C	4.8520	95.24867	-1404.03767	33.86500	-1370.17267	-1274.92400
6	H	-3.6083	26.43633	262.60877	0.32370	262.93247	289.36880
7	C	4.8523	95.25700	-1404.13413	33.85047	-1370.28366	-1275.02666
8	H	-3.6070	26.43600	262.51173	0.32325	262.83497	289.27097
9	C	4.8493	95.26233	-1403.26601	33.83458	-1369.43143	-1274.16909
10	H	-3.6073	26.43600	262.53599	0.32418	262.86017	289.29617

11	C	4.8497	95.25600	-1403.36246	33.84554	-1369.51692	-1274.26092
12	H	-3.6063	26.43633	262.46321	0.32390	262.78711	289.22344
13	C	4.8503	95.26433	-1403.55538	33.83344	-1369.72194	-1274.45760
14	H	-3.6093	26.43567	262.68154	0.32374	263.00528	289.44095
15	C	4.8523	95.24333	-1404.13413	33.87113	-1370.26300	-1275.01966
16	H	-3.6100	26.43567	262.73006	0.32481	263.05487	289.49054
17	C	4.8527	95.23567	-1404.23058	33.87637	-1370.35422	-1275.11855
18	H	-3.6083	26.43600	262.60877	0.32287	262.93163	289.36763
19	C	4.8520	95.24733	-1404.03767	33.85083	-1370.18684	-1274.93951
20	C	4.8507	95.26633	-1403.65184	33.82330	-1369.82854	-1274.56220
21	H	-3.6060	26.43633	262.43895	0.32353	262.76248	289.19882
ring 1H		-3.6082	26.43597	262.59664	0.32373	262.92037	289.35633
ring 13C		4.8514	95.25257	-1403.85440	33.85116	-1370.00323	-1274.75067

=====

3NiCp2-STO-PBE0-No-G

Temperature: 298

Spin: 1

atensor 1 Ni

122.260 0.000 0.005
0.000 122.260 0.006
0.005 0.006 17.302
-45.769 0.001 -0.004
0.001 -45.769 -0.003
-0.004 -0.003 -2.544

atensor 2 H

-6.721 -2.464 -1.066
-2.464 -0.665 2.999
-1.067 2.999 -3.334
-0.144 -0.069 -0.082
-0.069 0.026 0.231
-0.009 0.025 0.010

atensor 3 C

0.959 -0.328 -0.995
-0.328 1.765 2.798
-0.995 2.798 12.359
-0.302 -0.036 -0.068
-0.036 -0.214 0.192
-0.006 0.017 -0.010

atensor 4 H

0.205 0.214 -3.182
0.214 -7.591 -0.087
-3.182 -0.087 -3.335
0.051 0.006 -0.245
0.006 -0.169 -0.007
-0.026 -0.001 0.010

atensor 5 C

1.880 0.029 -2.969
0.029 0.843 -0.081
-2.969 -0.081 12.359
-0.201 0.003 -0.204
0.003 -0.315 -0.006
-0.018 -0.001 -0.010

atensor 6 H

-6.971 2.118 -0.900
2.118 -0.412 -3.054
-0.901 -3.054 -3.334
-0.151 0.060 -0.069
0.060 0.033 -0.236
-0.007 -0.025 0.010

atensor 7 C
0.927 0.282 -0.840
0.282 1.800 -2.849
-0.840 -2.849 12.356
-0.306 0.031 -0.058
0.031 -0.210 -0.196
-0.005 -0.018 -0.010

atensor 8 H
-2.283 -3.640 2.626
-3.640 -5.098 -1.800
2.626 -1.800 -3.332
-0.019 -0.103 0.203
-0.103 -0.099 -0.139
0.022 -0.015 0.010

atensor 9 C
1.550 -0.485 2.450
-0.485 1.175 -1.679
2.450 -1.679 12.350
-0.238 -0.053 0.168
-0.053 -0.279 -0.115
0.015 -0.010 -0.010

atensor 10 H
-2.690 3.773 2.523
3.773 -4.692 1.941
2.523 1.941 -3.332
-0.031 0.106 0.195
0.106 -0.087 0.150
0.021 0.016 0.010

atensor 11 C
1.495 0.502 2.354
0.502 1.228 1.811
2.354 1.811 12.353
-0.244 0.055 0.162
0.055 -0.273 0.124
0.015 0.011 -0.010

atensor 12 H
-6.968 2.117 0.901
2.117 -0.412 3.054
0.901 3.054 -3.331
-0.151 0.060 0.069
0.060 0.033 0.236
0.007 0.025 0.010

atensor 13 C
0.927 0.282 0.840
0.282 1.799 2.847
0.840 2.847 12.351
-0.306 0.031 0.058
0.031 -0.210 0.196
0.005 0.018 -0.010

atensor 14 H
-2.285 -3.641 -2.626
-3.641 -5.101 1.799
-2.626 1.800 -3.334
-0.019 -0.102 -0.203
-0.102 -0.099 0.139
-0.022 0.015 0.010

atensor 15 C
1.549 -0.484 -2.449

-0.484 1.174 1.677
-2.449 1.677 12.361
-0.238 -0.053 -0.168
-0.053 -0.279 0.115
-0.015 0.010 -0.010

atensor 16 H
-2.693 3.774 -2.522
3.774 -4.694 -1.941
-2.522 -1.941 -3.335
-0.031 0.106 -0.195
0.106 -0.087 -0.150
-0.021 -0.016 0.010

atensor 17 C
1.494 0.502 -2.353
0.502 1.228 -1.811
-2.353 -1.811 12.362
-0.243 0.055 -0.162
0.055 -0.273 -0.124
-0.015 -0.011 -0.010

atensor 18 H
-6.719 -2.464 1.066
-2.464 -0.664 -2.999
1.066 -2.999 -3.334
-0.144 -0.069 0.082
-0.069 0.026 -0.231
0.009 -0.025 0.010

atensor 19 C
0.960 -0.328 0.995
-0.328 1.766 -2.798
0.995 -2.799 12.356
-0.302 -0.036 0.068
-0.036 -0.214 -0.192
0.006 -0.017 -0.010

atensor 20 C
1.883 0.028 2.969
0.028 0.846 0.080
2.969 0.080 12.349
-0.201 0.003 0.204
0.003 -0.315 0.006
0.018 0.000 -0.010

atensor 21 H
0.207 0.214 3.183
0.214 -7.586 0.087
3.183 0.087 -3.331
0.051 0.006 0.246
0.006 -0.169 0.007
0.026 0.001 0.010

orbtensor 1 Ni
-11847.878 0.157 -0.449
0.157 -11847.827 -0.662
-0.449 -0.662 -383.621
2258.651 0.000 0.002
0.000 2258.651 -0.001
0.002 -0.001 2270.700

orbtensor 2 H
-0.535 5.101 0.750
5.101 -13.067 -2.110
0.750 -2.110 -0.262
27.938 -4.921 -0.778

-4.921 40.030 2.189
-0.778 2.189 25.203

orbtensor 3 C
-175.770 15.004 6.987
15.004 -212.618 -19.648
6.987 -19.648 -65.386
256.329 2.459 -1.435
2.459 250.284 4.033
-1.435 4.033 232.895

orbtensor 4 H
-14.869 -0.443 2.238
-0.443 1.267 0.062
2.238 0.062 -0.262
41.768 0.428 -2.321
0.428 26.200 -0.064
-2.321 -0.064 25.203

orbtensor 5 C
-217.917 -1.302 20.841
-1.302 -170.464 0.567
20.841 0.567 -65.382
249.417 -0.214 -4.279
-0.214 257.198 -0.116
-4.279 -0.116 232.894

orbtensor 6 H
-0.013 -4.384 0.633
-4.384 -13.587 2.147
0.633 2.147 -0.262
27.435 4.229 -0.657
4.229 40.533 -2.228
-0.657 -2.228 25.203

orbtensor 7 C
-174.212 -12.898 5.897
-12.898 -214.139 19.989
5.897 19.989 -65.383
256.578 -2.114 -1.212
-2.114 250.032 -4.105
-1.212 -4.105 232.895

orbtensor 8 H
-9.714 7.536 -1.847
7.536 -3.886 1.266
-1.847 1.266 -0.262
36.795 -7.271 1.916
-7.271 31.172 -1.313
1.916 -1.313 25.203

orbtensor 9 C
-202.736 22.169 -17.191
22.169 -185.594 11.781
-17.191 11.781 -65.384
251.898 3.634 3.531
3.634 254.708 -2.420
3.531 -2.420 232.895

orbtensor 10 H
-8.871 -7.810 -1.775
-7.810 -4.729 -1.365
-1.775 -1.365 -0.262
35.982 7.535 1.841
7.535 31.985 1.416
1.841 1.416 25.203

orbtensor 11 C
-200.262 -22.969 -16.521
-22.969 -188.087 -12.715
-16.521 -12.715 -65.384
252.304 -3.766 3.392
-3.766 254.303 2.612
3.392 2.612 232.894

orbtensor 12 H
-0.013 -4.383 -0.634
-4.383 -13.587 -2.150
-0.634 -2.150 -0.262
27.435 4.229 0.657
4.229 40.532 2.230
0.657 2.230 25.204

orbtensor 13 C
-174.196 -12.892 -5.887
-12.892 -214.126 -20.020
-5.887 -20.020 -65.387
256.577 -2.114 1.206
-2.114 250.029 4.109
1.206 4.109 232.896

orbtensor 14 H
-9.715 7.535 1.849
7.535 -3.887 -1.267
1.849 -1.267 -0.262
36.796 -7.270 -1.918
-7.270 31.172 1.314
-1.918 1.314 25.203

orbtensor 15 C
-202.768 22.158 17.227
22.158 -185.621 -11.805
17.227 -11.805 -65.390
251.901 3.635 -3.535
3.635 254.713 2.420
-3.535 2.420 232.895

orbtensor 16 H
-8.873 -7.809 1.776
-7.809 -4.730 1.366
1.776 1.366 -0.262
35.983 7.535 -1.842
7.535 31.986 -1.417
-1.842 -1.417 25.203

orbtensor 17 C
-200.301 -22.962 16.551
-22.962 -188.120 12.717
16.551 12.717 -65.382
252.309 -3.767 -3.396
-3.767 254.308 -2.608
-3.396 -2.608 232.893

orbtensor 18 H
-0.534 5.100 -0.750
5.100 -13.067 2.110
-0.750 2.110 -0.262
27.938 -4.921 0.777
-4.921 40.030 -2.188
0.777 -2.188 25.203

orbtensor 19 C
-175.756 14.996 -6.975
14.996 -212.624 19.650

```

-6.975   19.650  -65.384
256.328   2.460   1.429
2.460  250.284  -4.034
1.429   -4.034  232.894

```

```

orbtensor 20 C
-217.890  -1.297  -20.840
-1.297 -170.425  -0.578
-20.840  -0.578  -65.385
249.411  -0.215   4.279
-0.215  257.193   0.118
4.279    0.118  232.895

```

```

orbtensor 21 H
-14.867  -0.443  -2.239
-0.443   1.268  -0.061
-2.239  -0.061  -0.262
41.767   0.427   2.322
0.427   26.200   0.064
2.322   0.064  25.203

```

```

gtensor (ppt)
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.9133	-5763.77467	44140.89870	0.00000	44140.89870	38377.12403
2	H	-3.6093	26.43567	255.06846	-0.00000	255.06846	281.50413
3	C	4.8523	95.24467	-1363.44404	0.00000	-1363.44404	-1268.19937
4	H	-3.6097	26.43567	255.09202	0.00000	255.09202	281.52768
5	C	4.8520	95.24867	-1363.35038	0.00000	-1363.35038	-1268.10171
6	H	-3.6083	26.43633	254.99779	-0.00000	254.99779	281.43412
7	C	4.8523	95.25700	-1363.44404	0.00000	-1363.44404	-1268.18704
8	H	-3.6070	26.43600	254.90356	-0.00000	254.90356	281.33956
9	C	4.8493	95.26233	-1362.60108	0.00000	-1362.60108	-1267.33875
10	H	-3.6073	26.43600	254.92712	0.00000	254.92712	281.36312
11	C	4.8497	95.25600	-1362.69474	0.00000	-1362.69474	-1267.43874
12	H	-3.6063	26.43633	254.85645	-0.00000	254.85645	281.29278
13	C	4.8503	95.26433	-1362.88207	0.00000	-1362.88207	-1267.61773
14	H	-3.6093	26.43567	255.06846	-0.00000	255.06846	281.50413
15	C	4.8523	95.24333	-1363.44404	0.00000	-1363.44404	-1268.20071
16	H	-3.6100	26.43567	255.11557	-0.00000	255.11557	281.55124
17	C	4.8527	95.23567	-1363.53770	0.00000	-1363.53770	-1268.30204
18	H	-3.6083	26.43600	254.99779	0.00000	254.99779	281.43379
19	C	4.8520	95.24733	-1363.35038	0.00000	-1363.35038	-1268.10304
20	C	4.8507	95.26633	-1362.97573	0.00000	-1362.97573	-1267.70939
21	H	-3.6060	26.43633	254.83289	-0.00000	254.83289	281.26923
13C Average		4.8514	95.25257	-1363.17242	0.00000	-1363.17242	-1267.91985
1H Average		-3.6082	26.43597	254.98601	-0.00000	254.98601	281.42198

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3NiCp2-STO-PBE0-No-PSO
Temperature: 298
Spin: 1

```

atensor 1 Ni
122.260 0.000 0.005
0.000 122.260 0.006
0.005 0.006 17.302
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 2 H
-6.721 -2.464 -1.066
-2.464 -0.665 2.999
-1.067 2.999 -3.334
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
0.959 -0.328 -0.995
-0.328 1.765 2.798
-0.995 2.798 12.359
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 H
0.205 0.214 -3.182
0.214 -7.591 -0.087
-3.182 -0.087 -3.335
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
1.880 0.029 -2.969
0.029 0.843 -0.081
-2.969 -0.081 12.359
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H
-6.971 2.118 -0.900
2.118 -0.412 -3.054
-0.901 -3.054 -3.334
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
0.927 0.282 -0.840
0.282 1.800 -2.849
-0.840 -2.849 12.356
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-2.283 -3.640 2.626
-3.640 -5.098 -1.800
2.626 -1.800 -3.332
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
1.550 -0.485 2.450
-0.485 1.175 -1.679

2.450 -1.679 12.350
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-2.690 3.773 2.523
3.773 -4.692 1.941
2.523 1.941 -3.332
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
1.495 0.502 2.354
0.502 1.228 1.811
2.354 1.811 12.353
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
-6.968 2.117 0.901
2.117 -0.412 3.054
0.901 3.054 -3.331
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
0.927 0.282 0.840
0.282 1.799 2.847
0.840 2.847 12.351
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
-2.285 -3.641 -2.626
-3.641 -5.101 1.799
-2.626 1.800 -3.334
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
1.549 -0.484 -2.449
-0.484 1.174 1.677
-2.449 1.677 12.361
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 H
-2.693 3.774 -2.522
3.774 -4.694 -1.941
-2.522 -1.941 -3.335
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
1.494 0.502 -2.353
0.502 1.228 -1.811
-2.353 -1.811 12.362
0.000 0.000 0.000
0.000 0.000 0.000

0.000 0.000 0.000

atensor 18 H

-6.719 -2.464 1.066
-2.464 -0.664 -2.999
1.066 -2.999 -3.334
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C

0.960 -0.328 0.995
-0.328 1.766 -2.798
0.995 -2.799 12.356
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C

1.883 0.028 2.969
0.028 0.846 0.080
2.969 0.080 12.349
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H

0.207 0.214 3.183
0.214 -7.586 0.087
3.183 0.087 -3.331
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Ni

-11847.878 0.157 -0.449
0.157-11847.827 -0.662
-0.449 -0.662 -383.621
2258.651 0.000 0.002
0.000 2258.651 -0.001
0.002 -0.001 2270.700

orbtensor 2 H

-0.535 5.101 0.750
5.101 -13.067 -2.110
0.750 -2.110 -0.262
27.938 -4.921 -0.778
-4.921 40.030 2.189
-0.778 2.189 25.203

orbtensor 3 C

-175.770 15.004 6.987
15.004 -212.618 -19.648
6.987 -19.648 -65.386
256.329 2.459 -1.435
2.459 250.284 4.033
-1.435 4.033 232.895

orbtensor 4 H

-14.869 -0.443 2.238
-0.443 1.267 0.062
2.238 0.062 -0.262
41.768 0.428 -2.321
0.428 26.200 -0.064
-2.321 -0.064 25.203

orbtensor 5 C

-217.917	-1.302	20.841
-1.302	-170.464	0.567
20.841	0.567	-65.382
249.417	-0.214	-4.279
-0.214	257.198	-0.116
-4.279	-0.116	232.894

orbtensor 6 H

-0.013	-4.384	0.633
-4.384	-13.587	2.147
0.633	2.147	-0.262
27.435	4.229	-0.657
4.229	40.533	-2.228
-0.657	-2.228	25.203

orbtensor 7 C

-174.212	-12.898	5.897
-12.898	-214.139	19.989
5.897	19.989	-65.383
256.578	-2.114	-1.212
-2.114	250.032	-4.105
-1.212	-4.105	232.895

orbtensor 8 H

-9.714	7.536	-1.847
7.536	-3.886	1.266
-1.847	1.266	-0.262
36.795	-7.271	1.916
-7.271	31.172	-1.313
1.916	-1.313	25.203

orbtensor 9 C

-202.736	22.169	-17.191
22.169	-185.594	11.781
-17.191	11.781	-65.384
251.898	3.634	3.531
3.634	254.708	-2.420
3.531	-2.420	232.895

orbtensor 10 H

-8.871	-7.810	-1.775
-7.810	-4.729	-1.365
-1.775	-1.365	-0.262
35.982	7.535	1.841
7.535	31.985	1.416
1.841	1.416	25.203

orbtensor 11 C

-200.262	-22.969	-16.521
-22.969	-188.087	-12.715
-16.521	-12.715	-65.384
252.304	-3.766	3.392
-3.766	254.303	2.612
3.392	2.612	232.894

orbtensor 12 H

-0.013	-4.383	-0.634
-4.383	-13.587	-2.150
-0.634	-2.150	-0.262
27.435	4.229	0.657
4.229	40.532	2.230
0.657	2.230	25.204

orbtensor 13 C

-174.196	-12.892	-5.887
-12.892	-214.126	-20.020
-5.887	-20.020	-65.387

256.577	-2.114	1.206
-2.114	250.029	4.109
1.206	4.109	232.896

orbtensor 14 H

-9.715	7.535	1.849
7.535	-3.887	-1.267
1.849	-1.267	-0.262
36.796	-7.270	-1.918
-7.270	31.172	1.314
-1.918	1.314	25.203

orbtensor 15 C

-202.768	22.158	17.227
22.158	-185.621	-11.805
17.227	-11.805	-65.390
251.901	3.635	-3.535
3.635	254.713	2.420
-3.535	2.420	232.895

orbtensor 16 H

-8.873	-7.809	1.776
-7.809	-4.730	1.366
1.776	1.366	-0.262
35.983	7.535	-1.842
7.535	31.986	-1.417
-1.842	-1.417	25.203

orbtensor 17 C

-200.301	-22.962	16.551
-22.962	-188.120	12.717
16.551	12.717	-65.382
252.309	-3.767	-3.396
-3.767	254.308	-2.608
-3.396	-2.608	232.893

orbtensor 18 H

-0.534	5.100	-0.750
5.100	-13.067	2.110
-0.750	2.110	-0.262
27.938	-4.921	0.777
-4.921	40.030	-2.188
0.777	-2.188	25.203

orbtensor 19 C

-175.756	14.996	-6.975
14.996	-212.624	19.650
-6.975	19.650	-65.384
256.328	2.460	1.429
2.460	250.284	-4.034
1.429	-4.034	232.894

orbtensor 20 C

-217.890	-1.297	-20.840
-1.297	-170.425	-0.578
-20.840	-0.578	-65.385
249.411	-0.215	4.279
-0.215	257.193	0.118
4.279	0.118	232.895

orbtensor 21 H

-14.867	-0.443	-2.239
-0.443	1.268	-0.061
-2.239	-0.061	-0.262
41.767	0.427	2.322
0.427	26.200	0.064
2.322	0.064	25.203


```

gtensor (ppt)
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	87.2740	-5763.77467	68898.64302	0.00000	68898.64302	63134.86835
2	H	-3.5733	26.43567	252.52437	-0.00000	252.52437	278.96004
3	C	5.0277	95.24467	-1412.71048	0.00000	-1412.71048	-1317.46581
4	H	-3.5737	26.43567	252.54793	-0.00000	252.54793	278.98359
5	C	5.0273	95.24867	-1412.61682	0.00000	-1412.61682	-1317.36815
6	H	-3.5723	26.43633	252.45370	0.00000	252.45370	278.89003
7	C	5.0277	95.25700	-1412.71048	0.00000	-1412.71048	-1317.45348
8	H	-3.5710	26.43600	252.35948	-0.00000	252.35948	278.79548
9	C	5.0250	95.26233	-1411.96118	0.00000	-1411.96118	-1316.69885
10	H	-3.5713	26.43600	252.38303	0.00000	252.38303	278.81903
11	C	5.0253	95.25600	-1412.05484	0.00000	-1412.05484	-1316.79884
12	H	-3.5703	26.43633	252.31236	-0.00000	252.31236	278.74870
13	C	5.0257	95.26433	-1412.14851	0.00000	-1412.14851	-1316.88417
14	H	-3.5733	26.43567	252.52437	-0.00000	252.52437	278.96004
15	C	5.0280	95.24333	-1412.80414	-0.00000	-1412.80414	-1317.56081
16	H	-3.5740	26.43567	252.57148	-0.00000	252.57148	279.00715
17	C	5.0280	95.23567	-1412.80414	0.00000	-1412.80414	-1317.56848
18	H	-3.5723	26.43600	252.45370	0.00000	252.45370	278.88970
19	C	5.0273	95.24733	-1412.61682	0.00000	-1412.61682	-1317.36948
20	C	5.0260	95.26633	-1412.24217	0.00000	-1412.24217	-1316.97583
21	H	-3.5700	26.43633	252.28881	-0.00000	252.28881	278.72514
13C Average		5.0268	95.25257	-1412.46696	0.00000	-1412.46696	-1317.21439
1H Average		-3.5722	26.43597	252.44192	-0.00000	252.44192	278.87789

3NiCp2-STO-PBE0-No-ZORA

Temperature: 298

Spin: 1

```

atensor 2 H
-6.810 -2.482 -1.053
-2.482 -0.712 2.963
-1.054 2.963 -3.417
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

```

```

atensor 3 C
0.760 -0.325 -0.992
-0.325 1.560 2.789
-0.992 2.789 12.403
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

```

```

atensor 4 H
0.165 0.216 -3.143
0.216 -7.687 -0.086
-3.143 -0.086 -3.418

```

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
1.674 0.028 -2.960
0.028 0.645 -0.081
-2.960 -0.081 12.403
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H
-7.062 2.132 -0.889
2.132 -0.457 -3.016
-0.890 -3.017 -3.417
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
0.728 0.280 -0.837
0.280 1.595 -2.840
-0.837 -2.840 12.400
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-2.341 -3.666 2.594
-3.666 -5.176 -1.778
2.594 -1.778 -3.415
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
1.347 -0.481 2.442
-0.481 0.975 -1.674
2.442 -1.674 12.395
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-2.751 3.799 2.492
3.799 -4.767 1.918
2.493 1.918 -3.415
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
1.292 0.498 2.346
0.498 1.027 1.805
2.347 1.805 12.397
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
-7.060 2.132 0.890
2.132 -0.458 3.017
0.890 3.017 -3.414
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
0.729 0.280 0.838
0.280 1.594 2.838
0.838 2.838 12.395
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
-2.344 -3.666 -2.594
-3.666 -5.179 1.777
-2.594 1.778 -3.417
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
1.345 -0.480 -2.441
-0.480 0.974 1.672
-2.441 1.672 12.404
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 H
-2.754 3.800 -2.491
3.800 -4.769 -1.917
-2.492 -1.917 -3.417
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
1.291 0.498 -2.345
0.498 1.027 -1.806
-2.345 -1.806 12.406
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 H
-6.808 -2.482 1.053
-2.482 -0.711 -2.963
1.053 -2.963 -3.416
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
0.761 -0.326 0.992
-0.326 1.561 -2.790
0.992 -2.790 12.400
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C
1.678 0.028 2.959
0.028 0.648 0.080
2.959 0.080 12.394
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H
0.166 0.215 3.144

0.215 -7.682 0.086
3.144 0.086 -3.414
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 2 H

-0.613 5.073 0.731
5.073 -13.078 -2.057
0.731 -2.057 -0.262
27.956 -4.923 -0.777
-4.923 40.052 2.184
-0.777 2.184 25.211

orbtensor 3 C

-176.623 15.126 6.842
15.126 -213.772 -19.242
6.842 -19.242 -65.382
256.590 2.462 -1.424
2.462 250.539 4.003
-1.424 4.003 233.072

orbtensor 4 H

-14.870 -0.441 2.182
-0.441 1.179 0.060
2.182 0.060 -0.261
41.791 0.428 -2.316
0.428 26.217 -0.063
-2.316 -0.063 25.210

orbtensor 5 C

-219.114 -1.313 20.410
-1.313 -171.274 0.556
20.410 0.556 -65.378
249.670 -0.214 -4.246
-0.214 257.459 -0.115
-4.246 -0.115 233.072

orbtensor 6 H

-0.094 -4.360 0.617
-4.360 -13.596 2.093
0.617 2.093 -0.261
27.453 4.231 -0.655
4.231 40.555 -2.222
-0.655 -2.222 25.210

orbtensor 7 C

-175.052 -13.003 5.775
-13.003 -215.306 19.575
5.775 19.575 -65.379
256.839 -2.116 -1.203
-2.116 250.286 -4.074
-1.203 -4.074 233.072

orbtensor 8 H

-9.743 7.496 -1.800
7.496 -3.946 1.234
-1.800 1.234 -0.261
36.816 -7.274 1.911
-7.274 31.191 -1.310
1.911 -1.310 25.210

orbtensor 9 C

-203.810 22.350 -16.835
22.350 -186.527 11.537
-16.835 11.537 -65.380
252.154 3.638 3.504

3.638 254.968 -2.401
3.504 -2.401 233.073

orbtensor 10 H
-8.905 -7.768 -1.730
-7.768 -4.784 -1.331
-1.730 -1.331 -0.261
36.003 7.538 1.836
7.538 32.004 1.413
1.836 1.413 25.211

orbtensor 11 C
-201.316 -23.157 -16.179
-23.157 -189.041 -12.452
-16.179 -12.452 -65.380
252.561 -3.770 3.366
-3.770 254.562 2.592
3.366 2.592 233.072

orbtensor 12 H
-0.094 -4.360 -0.618
-4.360 -13.595 -2.096
-0.618 -2.096 -0.262
27.453 4.231 0.655
4.231 40.555 2.224
0.655 2.224 25.211

orbtensor 13 C
-175.036 -12.998 -5.765
-12.998 -215.293 -19.606
-5.765 -19.606 -65.383
256.838 -2.116 1.197
-2.116 250.283 4.078
1.197 4.078 233.074

orbtensor 14 H
-9.744 7.495 1.803
7.495 -3.947 -1.236
1.803 -1.236 -0.262
36.817 -7.273 -1.914
-7.273 31.191 1.311
-1.914 1.311 25.211

orbtensor 15 C
-203.841 22.340 16.872
22.340 -186.555 -11.561
16.872 -11.561 -65.386
252.157 3.639 -3.508
3.639 254.972 2.401
-3.508 2.401 233.072

orbtensor 16 H
-8.906 -7.767 1.731
-7.767 -4.786 1.332
1.731 1.332 -0.261
36.004 7.538 -1.838
7.538 32.005 -1.413
-1.838 -1.413 25.210

orbtensor 17 C
-201.354 -23.150 16.209
-23.150 -189.074 12.454
16.209 12.454 -65.378
252.566 -3.770 -3.370
-3.770 254.567 -2.588
-3.370 -2.588 233.071

```

orbtensor 18 H
-0.613   5.073  -0.731
5.073  -13.078  2.057
-0.731   2.057  -0.261
27.956  -4.923   0.775
-4.923  40.053  -2.183
0.775   -2.183  25.210

```

```

orbtensor 19 C
-176.609  15.119  -6.830
15.119 -213.778  19.244
-6.830  19.244  -65.380
256.588   2.462   1.418
2.462  250.538  -4.003
1.418   -4.003  233.072

```

```

orbtensor 20 C
-219.088  -1.308  -20.408
-1.308 -171.235  -0.566
-20.408  -0.566  -65.381
249.665  -0.215   4.246
-0.215  257.454   0.117
4.246   0.117  233.073

```

```

orbtensor 21 H
-14.869  -0.440  -2.182
-0.440   1.180  -0.060
-2.182  -0.060  -0.262
41.790   0.427   2.316
0.427  26.217   0.064
2.316   0.064  25.211

```

```

gtensor (ppt)
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	-3.6463	26.42200	257.68346	-0.00000	257.68346	284.10546
3	C	4.9077	94.80800	-1378.98847	0.00000	-1378.98847	-1284.18047
4	H	-3.6467	26.42200	257.70702	-0.00000	257.70702	284.12902
5	C	4.9073	94.81167	-1378.89481	0.00000	-1378.89481	-1284.08314
6	H	-3.6453	26.42233	257.61279	-0.00000	257.61279	284.03513
7	C	4.9077	94.82000	-1378.98847	0.00000	-1378.98847	-1284.16847
8	H	-3.6440	26.42233	257.51857	0.00000	257.51857	283.94090
9	C	4.9057	94.82600	-1378.42650	0.00000	-1378.42650	-1283.60050
10	H	-3.6443	26.42267	257.54212	0.00000	257.54212	283.96479
11	C	4.9053	94.81933	-1378.33284	0.00000	-1378.33284	-1283.51350
12	H	-3.6440	26.42267	257.51857	-0.00000	257.51857	283.94123
13	C	4.9060	94.82767	-1378.52016	0.00000	-1378.52016	-1283.69249
14	H	-3.6467	26.42200	257.70702	0.00000	257.70702	284.12902
15	C	4.9077	94.80633	-1378.98847	0.00000	-1378.98847	-1284.18214
16	H	-3.6467	26.42200	257.70702	0.00000	257.70702	284.12902
17	C	4.9080	94.79933	-1379.08213	0.00000	-1379.08213	-1284.28280
18	H	-3.6450	26.42233	257.58924	-0.00000	257.58924	284.01157
19	C	4.9073	94.81033	-1378.89481	0.00000	-1378.89481	-1284.08447
20	C	4.9067	94.82933	-1378.70748	0.00000	-1378.70748	-1283.87815
21	H	-3.6433	26.42233	257.47145	0.00000	257.47145	283.89379

ring 1H	-3.6452	26.42227	257.60573	0.00000	257.60573	284.02799
ring 13C	4.9069	94.81580	-1378.78241	0.00000	-1378.78241	-1283.96661

=====
3NiCp2-GTO-B3LYP
Temperature: 298
Spin: 1

atensor 1 Ni
104.5614 -0.0005 0.0049
-0.0005 104.5616 0.0054
0.0049 0.0054 2.6349
-38.6185 0.0001 -0.0033
0.0001 -38.6185 -0.0021
-0.0033 -0.0021 -2.9584

atensor 2 H
-6.5084 -2.5624 -1.0276
-2.5624 -0.2117 2.8899
-1.0276 2.8899 -3.3191
-0.1225 -0.0560 -0.0387
-0.0560 0.0151 0.1089
-0.0387 0.1089 0.0111

atensor 3 C
0.8611 -0.3201 -0.9717
-0.3201 1.6478 2.7331
-0.9717 2.7331 13.6239
-0.2780 -0.0317 -0.0332
-0.0317 -0.2001 0.0933
-0.0332 0.0933 -0.0119

atensor 4 H
0.6932 0.2228 -3.0659
0.2228 -7.4139 -0.0842
-3.0659 -0.0842 -3.3199
0.0349 0.0049 -0.1155
0.0049 -0.1423 -0.0032
-0.1155 -0.0032 0.0111

atensor 5 C
1.7606 0.0279 -2.9003
0.0279 0.7477 -0.0798
-2.9003 -0.0798 13.6247
-0.1889 0.0027 -0.0990
0.0027 -0.2893 -0.0027
-0.0990 -0.0027 -0.0119

atensor 6 H
-6.7686 2.2017 -0.8676
2.2017 0.0509 -2.9422
-0.8676 -2.9422 -3.3185
-0.1283 0.0482 -0.0327
0.0482 0.0208 -0.1109
-0.0327 -0.1109 0.0111

atensor 7 C
0.8290 0.2751 -0.8204
0.2751 1.6814 -2.7828
-0.8204 -2.7828 13.6186
-0.2814 0.0273 -0.0280
0.0273 -0.1969 -0.0950
-0.0280 -0.0950 -0.0119

atensor 8 H
-1.8943 -3.7851 2.5303
-3.7851 -4.8220 -1.7345

2.5303 -1.7345 -3.3173
-0.0217 -0.0828 0.0953
-0.0828 -0.0858 -0.0654
0.0953 -0.0654 0.0111

atensor 9 C
1.4378 -0.4731 2.3927
-0.4731 1.0718 -1.6402
2.3927 -1.6402 13.6143
-0.2209 -0.0470 0.0817
-0.0470 -0.2573 -0.0560
0.0817 -0.0560 -0.0119

atensor 10 H
-2.3178 3.9228 2.4312
3.9228 -4.3995 1.8705
2.4312 1.8705 -3.3175
-0.0310 0.0858 0.0916
0.0858 -0.0765 0.0705
0.0916 0.0705 0.0111

atensor 11 C
1.3840 0.4902 2.2991
0.4902 1.1236 1.7687
2.2991 1.7687 13.6162
-0.2262 0.0486 0.0785
0.0486 -0.2520 0.0604
0.0785 0.0604 -0.0119

atensor 12 H
-6.7668 2.2018 0.8678
2.2018 0.0502 2.9428
0.8678 2.9428 -3.3165
-0.1283 0.0482 0.0327
0.0482 0.0208 0.1109
0.0327 0.1109 0.0111

atensor 13 C
0.8298 0.2754 0.8209
0.2754 1.6812 2.7807
0.8209 2.7807 13.6151
-0.2814 0.0273 0.0280
0.0273 -0.1968 0.0950
0.0280 0.0950 -0.0119

atensor 14 H
-1.8966 -3.7857 -2.5303
-3.7857 -4.8243 1.7339
-2.5303 1.7339 -3.3186
-0.0218 -0.0827 -0.0953
-0.0827 -0.0858 0.0653
-0.0953 0.0653 0.0111

atensor 15 C
1.4365 -0.4727 -2.3915
-0.4727 1.0710 1.6383
-2.3915 1.6383 13.6248
-0.2209 -0.0468 -0.0817
-0.0468 -0.2573 0.0560
-0.0817 0.0560 -0.0119

atensor 16 H
-2.3201 3.9238 -2.4304
3.9238 -4.4010 -1.8701
-2.4304 -1.8701 -3.3196
-0.0310 0.0857 -0.0916
0.0857 -0.0765 -0.0704

-0.0916 -0.0704 0.0111

atensor 17 C

1.3833 0.4902 -2.2978
0.4902 1.1238 -1.7694
-2.2978 -1.7694 13.6265
-0.2262 0.0485 -0.0785
0.0485 -0.2519 -0.0604
-0.0785 -0.0604 -0.0119

atensor 18 H

-6.5068 -2.5625 1.0272
-2.5625 -0.2113 -2.8899
1.0272 -2.8899 -3.3186
-0.1226 -0.0560 0.0387
-0.0560 0.0151 -0.1089
0.0387 -0.1089 0.0111

atensor 19 C

0.8618 -0.3205 0.9719
-0.3205 1.6486 -2.7335
0.9719 -2.7335 13.6200
-0.2781 -0.0317 0.0332
-0.0317 -0.2000 -0.0933
0.0332 -0.0933 -0.0119

atensor 20 C

1.7634 0.0276 2.8995
0.0276 0.7502 0.0783
2.8995 0.0783 13.6122
-0.1888 0.0027 0.0990
0.0027 -0.2894 0.0027
0.0990 0.0027 -0.0119

atensor 21 H

0.6943 0.2223 3.0667
0.2223 -7.4090 0.0837
3.0667 0.0837 -3.3164
0.0349 0.0048 0.1156
0.0048 -0.1424 0.0032
0.1156 0.0032 0.0111

orbtensor 1 Ni

2261.0644 -0.0002 0.0042
-0.0002 2261.0645 -0.0005
0.0042 -0.0005 2273.9475
-10401.5942 0.0597 -0.2799
0.0597 -10401.6273 -0.5548
-0.2799 -0.5548 -436.3147

orbtensor 2 H

25.6117 -5.7544 -0.5031
-5.7544 39.7508 1.4148
-0.5031 1.4148 24.3161
1.6986 5.7797 0.3157
5.7797 -12.5021 -0.8885
0.3157 -0.8885 0.5882

orbtensor 3 C

252.9954 0.3621 -0.1679
0.3621 252.1040 0.4715
-0.1679 0.4715 238.9551
-182.9154 18.0147 5.4979
18.0147 -227.1670 -15.4634
5.4979 -15.4634 -79.8183

orbtensor 4 H

41.7836 0.4998 -1.4999
0.4998 23.5795 -0.0411
-1.4999 -0.0411 24.3162
-14.5437 -0.5018 0.9416
-0.5018 3.7398 0.0260
0.9416 0.0260 0.5884

orbtensor 5 C
251.9778 -0.0317 -0.4993
-0.0317 253.1242 -0.0128
-0.4993 -0.0128 238.9559
-233.5349 -1.5630 16.4000
-1.5630 -176.5496 0.4464
16.4000 0.4464 -79.8168

orbtensor 6 H
25.0241 4.9456 -0.4242
4.9456 40.3395 -1.4387
-0.4242 -1.4387 24.3159
2.2890 -4.9671 0.2659
-4.9671 -13.0925 0.9030
0.2659 0.9030 0.5886

orbtensor 7 C
253.0354 -0.3111 -0.1414
-0.3111 252.0698 -0.4762
-0.1414 -0.4762 238.9569
-181.0551 -15.4870 4.6389
-15.4870 -228.9998 15.7260
4.6389 15.7260 -79.8171

orbtensor 8 H
35.9701 -8.5022 1.2371
-8.5022 29.3940 -0.8480
1.2371 -0.8480 24.3163
-8.7037 8.5391 -0.7763
8.5391 -2.0995 0.5322
-0.7763 0.5322 0.5885

orbtensor 9 C
252.3452 0.5356 0.4093
0.5356 252.7600 -0.2802
0.4093 -0.2802 238.9575
-215.3101 26.6183 -13.5227
26.6183 -194.7253 9.2671
-13.5227 9.2671 -79.8190

orbtensor 10 H
35.0188 8.8110 1.1893
8.8110 30.3446 0.9151
1.1893 0.9151 24.3164
-7.7486 -8.8493 -0.7468
-8.8493 -3.0543 -0.5742
-0.7468 -0.5742 0.5883

orbtensor 11 C
252.4034 -0.5550 0.3941
-0.5550 252.6990 0.3047
0.3941 0.3047 238.9570
-212.3360 -27.5798 -12.9992
-27.5798 -197.7136 -10.0050
-12.9992 -10.0050 -79.8178

orbtensor 12 H
25.0244 4.9454 0.4245
4.9454 40.3397 1.4410
0.4245 1.4410 24.3168

2.2896 -4.9668 -0.2671
-4.9668 -13.0922 -0.9048
-0.2671 -0.9048 0.5876

orbtensor 13 C
253.0332 -0.3115 0.1380
-0.3115 252.0700 0.4775
0.1380 0.4775 238.9581
-181.0372 -15.4793 -4.6331
-15.4793 -228.9901 -15.7538
-4.6331 -15.7538 -79.8205

orbtensor 14 H
35.9699 -8.5019 -1.2412
-8.5019 29.3938 0.8503
-1.2412 0.8503 24.3158
-8.7041 8.5386 0.7798
8.5386 -2.0994 -0.5346
0.7798 -0.5346 0.5882

orbtensor 15 C
252.3455 0.5346 -0.4153
0.5346 252.7582 0.2833
-0.4153 0.2833 238.9549
-215.3379 26.6096 13.5637
26.6096 -194.7441 -9.2969
13.5637 -9.2969 -79.8213

orbtensor 16 H
35.0190 8.8109 -1.1916
8.8109 30.3448 -0.9165
-1.1916 -0.9165 24.3154
-7.7492 -8.8492 0.7485
-8.8492 -3.0551 0.5762
0.7485 0.5762 0.5885

orbtensor 17 C
252.4045 -0.5538 -0.4004
-0.5538 252.6985 -0.3055
-0.4004 -0.3055 238.9541
-212.3718 -27.5742 13.0319
-27.5742 -197.7420 10.0120
13.0319 10.0120 -79.8150

orbtensor 18 H
25.6119 -5.7542 0.5022
-5.7542 39.7520 -1.4140
0.5022 -1.4140 24.3161
1.6989 5.7794 -0.3159
5.7794 -12.5026 0.8878
-0.3159 0.8878 0.5881

orbtensor 19 C
252.9956 0.3622 0.1648
0.3622 252.1063 -0.4706
0.1648 -0.4706 238.9560
-182.9000 18.0074 -5.4901
18.0074 -227.1708 15.4634
-5.4901 15.4634 -79.8168

orbtensor 20 C
251.9781 -0.0317 0.4944
-0.0317 253.1239 0.0140
0.4944 0.0140 238.9584
-233.5054 -1.5603 -16.3947
-1.5603 -176.5094 -0.4563
-16.3947 -0.4563 -79.8181

```

orbtensor 21 H
41.7839 0.4995 1.4996
0.4995 23.5798 0.0410
1.4996 0.0410 24.3167
-14.5428 -0.5016 -0.9414
-0.5016 3.7404 -0.0256
-0.9414 -0.0256 0.5877

```

```

gtensor (ppt)
0.0071 -0.0000 0.0000
-0.0000 0.0071 0.0000
0.0000 0.0000 -0.1286
71.9698 -0.0006 0.0057
-0.0006 71.9703 0.0042
0.0057 0.0042 0.9569

```

```

averaging
1H Average:2,4,6,8,10,12,14,16,18,21
13C Average:3,5,7,9,11,13,15,17,19,20

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	43.8542	-4814.48660	35455.21056	413.08732	35868.29788	31053.81128
2	H	-3.3785	26.48777	244.51050	0.05880	244.56931	271.05707
3	C	5.2143	84.71793	-1500.45244	27.94805	-1472.50439	-1387.78646
4	H	-3.3790	26.48793	244.54428	0.05919	244.60347	271.09141
5	C	5.2143	84.71887	-1500.46203	27.95286	-1472.50918	-1387.79031
6	H	-3.3775	26.48820	244.44054	0.05914	244.49968	270.98788
7	C	5.2129	84.73003	-1500.06876	27.93705	-1472.13172	-1387.40168
8	H	-3.3767	26.48857	244.37782	0.05876	244.43658	270.92515
9	C	5.2113	84.73610	-1499.58917	27.92601	-1471.66315	-1386.92705
10	H	-3.3771	26.48840	244.40677	0.05868	244.46545	270.95385
11	C	5.2112	84.73067	-1499.57957	27.93117	-1471.64840	-1386.91773
12	H	-3.3765	26.48863	244.36576	0.05910	244.42486	270.91349
13	C	5.2120	84.73783	-1499.80019	27.92534	-1471.87485	-1387.13702
14	H	-3.3787	26.48807	244.52257	0.05970	244.58226	271.07033
15	C	5.2141	84.71843	-1500.39489	27.95295	-1472.44194	-1387.72351
16	H	-3.3790	26.48780	244.54910	0.05963	244.60873	271.09653
17	C	5.2145	84.70943	-1500.52918	27.95844	-1472.57074	-1387.86130
18	H	-3.3777	26.48813	244.45261	0.05886	244.51146	270.99960
19	C	5.2135	84.72343	-1500.22224	27.93889	-1472.28335	-1387.55992
20	C	5.2119	84.74250	-1499.77141	27.91598	-1471.85543	-1387.11293
21	H	-3.3758	26.48857	244.31751	0.05863	244.37614	270.86471
	ring 1H	-3.3776	26.48821	244.44875	0.05905	244.50780	270.99600
	ring 13C	5.2130	84.72652	-1500.08699	27.93867	-1472.14831	-1387.42179

```

=====
3NiCp2-GTO-BHLYP
Temperature: 298
Spin: 1

```

```

atensor 2 H
-5.7935 -2.3455 -1.1865
-2.3455 -0.0299 3.3365
-1.1865 3.3365 -2.6200
-0.2253 -0.1197 -0.0672
-0.1197 0.0689 0.1891
-0.0672 0.1891 0.0064

```

```

atensor 3 C
2.6641 -0.4051 -1.0325
-0.4051 3.6592 2.9032
-1.0325 2.9032 12.2355

```

-0.3931 -0.0398 -0.0509
 -0.0398 -0.2954 0.1432
 -0.0509 0.1432 -0.0068

orbtensor 2 H
 25.4280 -5.7231 -0.5217
 -5.7231 39.4901 1.4672
 -0.5217 1.4672 24.2225
 4.3982 7.1753 1.0835
 7.1753 -13.2309 -3.0485
 1.0835 -3.0485 0.3631

orbtensor 3 C
 251.5591 0.3138 -0.3829
 0.3138 250.7865 1.0765
 -0.3829 1.0765 238.3093
 -167.3070 20.1356 8.2594
 20.1356 -216.7672 -23.2331
 8.2594 -23.2331 -71.7797

gtensor (ppt)
 -0.0342 0.0000 0.0000
 0.0000 -0.0342 0.0000
 0.0000 0.0000 -0.1561
 149.4277 -0.0006 -0.0029
 -0.0006 149.4282 0.0151
 -0.0029 0.0151 0.3589

averaging
 1H Average:2,4,6,8,10,12,14,16,18,21
 13C Average:3,5,7,9,11,13,15,17,19,20

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	-2.8645	26.89033	212.50530	0.43892	212.94422	239.83455
3	C	5.9545	94.93367	-1756.41318	43.78102	-1712.63217	-1617.69850
4	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
5	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
7	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
8	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
9	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
10	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
11	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
12	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
13	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
14	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
15	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
16	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
17	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
19	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
20	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
21	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
	ring 1H	-0.2864	2.68903	21.25053	0.04389	21.29442	23.98346
	ring 13C	0.5955	9.49337	-175.64132	4.37810	-171.26322	-161.76985

3NiCp2-GTO-BP
 Temperature: 298
 Spin: 1

atensor 1 Ni

87.2887 -0.0004 0.0103
-0.0004 87.2887 0.0061
0.0103 0.0061 -0.4128
-24.9641 0.0001 -0.0028
0.0001 -24.9641 -0.0012
-0.0028 -0.0012 -2.6752

atensor 2 H
-6.8571 -2.6646 -0.9105
-2.6646 -0.3092 2.5606
-0.9105 2.5606 -3.6264
-0.0785 -0.0294 -0.0258
-0.0294 -0.0063 0.0725
-0.0258 0.0725 0.0101

atensor 3 C
-1.3062 -0.2404 -0.8980
-0.2404 -0.7150 2.5261
-0.8980 2.5261 13.2800
-0.2170 -0.0302 -0.0262
-0.0302 -0.1429 0.0736
-0.0262 0.0736 -0.0112

atensor 4 H
0.6318 0.2316 -2.7165
0.2316 -7.7988 -0.0746
-2.7165 -0.0746 -3.6273
0.0041 0.0025 -0.0769
0.0025 -0.0889 -0.0021
-0.0769 -0.0021 0.0101

atensor 5 C
-0.6304 0.0210 -2.6808
0.0210 -1.3914 -0.0738
-2.6808 -0.0738 13.2811
-0.1322 0.0026 -0.0781
0.0026 -0.2277 -0.0021
-0.0781 -0.0021 -0.0112

atensor 6 H
-7.1284 2.2896 -0.7687
2.2896 -0.0367 -2.6068
-0.7687 -2.6068 -3.6264
-0.0816 0.0253 -0.0218
0.0253 -0.0032 -0.0738
-0.0218 -0.0738 0.0101

atensor 7 C
-1.3297 0.2066 -0.7581
0.2066 -0.6890 -2.5723
-0.7581 -2.5723 13.2757
-0.2201 0.0260 -0.0221
0.0260 -0.1398 -0.0749
-0.0221 -0.0749 -0.0112

atensor 8 H
-2.0594 -3.9360 2.2418
-3.9360 -5.1038 -1.5368
2.2418 -1.5368 -3.6250
-0.0256 -0.0435 0.0635
-0.0435 -0.0592 -0.0435
0.0635 -0.0435 0.0101

atensor 9 C
-0.8722 -0.3556 2.2116
-0.3556 -1.1472 -1.5160
2.2116 -1.5160 13.2703

-0.1627 -0.0446 0.0644
-0.0446 -0.1972 -0.0442
0.0644 -0.0442 -0.0112

atensor 10 H
-2.4996 4.0793 2.1541
4.0793 -4.6644 1.6573
2.1541 1.6573 -3.6251
-0.0304 0.0451 0.0610
0.0451 -0.0543 0.0469
0.0610 0.0469 0.0101

atensor 11 C
-0.9128 0.3684 2.1251
0.3684 -1.1086 1.6346
2.1251 1.6346 13.2729
-0.1677 0.0462 0.0619
0.0462 -0.1922 0.0476
0.0619 0.0476 -0.0112

atensor 12 H
-7.1255 2.2897 0.7689
2.2897 -0.0366 2.6075
0.7689 2.6075 -3.6237
-0.0816 0.0253 0.0218
0.0253 -0.0032 0.0738
0.0218 0.0738 0.0101

atensor 13 C
-1.3291 0.2070 0.7591
0.2070 -0.6896 2.5695
0.7591 2.5695 13.2708
-0.2202 0.0259 0.0221
0.0259 -0.1398 0.0749
0.0221 0.0749 -0.0112

atensor 14 H
-2.0612 -3.9369 -2.2420
-3.9369 -5.1056 1.5363
-2.2420 1.5363 -3.6259
-0.0256 -0.0434 -0.0635
-0.0434 -0.0592 0.0435
-0.0635 0.0435 0.0101

atensor 15 C
-0.8742 -0.3551 -2.2099
-0.3551 -1.1487 1.5140
-2.2099 1.5140 13.2817
-0.1627 -0.0445 -0.0644
-0.0445 -0.1972 0.0441
-0.0644 0.0441 -0.0112

atensor 16 H
-2.5017 4.0805 -2.1535
4.0805 -4.6657 -1.6571
-2.1535 -1.6571 -3.6269
-0.0305 0.0450 -0.0610
0.0450 -0.0543 -0.0469
-0.0610 -0.0469 0.0101

atensor 17 C
-0.9144 0.3683 -2.1234
0.3683 -1.1091 -1.6356
-2.1234 -1.6356 13.2835
-0.1677 0.0461 -0.0619
0.0461 -0.1922 -0.0476
-0.0619 -0.0476 -0.0112

atensor 18 H
-6.8560 -2.6649 0.9101
-2.6649 -0.3092 -2.5605
0.9101 -2.5605 -3.6263
-0.0785 -0.0294 0.0258
-0.0294 -0.0062 -0.0725
0.0258 -0.0725 0.0101

atensor 19 C
-1.3052 -0.2409 0.8986
-0.2409 -0.7141 -2.5265
0.8986 -2.5265 13.2772
-0.2170 -0.0302 0.0262
-0.0302 -0.1428 -0.0736
0.0262 -0.0736 -0.0112

atensor 20 C
-0.6272 0.0208 2.6799
0.0208 -1.3887 0.0722
2.6799 0.0722 13.2687
-0.1321 0.0026 0.0781
0.0026 -0.2278 0.0021
0.0781 0.0021 -0.0112

atensor 21 H
0.6327 0.2312 2.7171
0.2312 -7.7940 0.0741
2.7171 0.0741 -3.6240
0.0042 0.0025 0.0769
0.0025 -0.0890 0.0021
0.0769 0.0021 0.0101

orbtensor 1 Ni
2268.6446 -0.0002 0.0048
-0.0002 2268.6448 -0.0002
0.0048 -0.0002 2273.4606
-7586.5070 0.0422 -0.1413
0.0422 -7586.5196 -0.3296
-0.1413 -0.3296 -642.3345

orbtensor 2 H
25.4292 -6.0735 -0.6166
-6.0735 40.3522 1.7343
-0.6166 1.7343 24.1075
0.7398 5.5446 0.1498
5.5446 -12.8831 -0.4217
0.1498 -0.4217 0.7841

orbtensor 3 C
255.4181 0.6774 -0.2391
0.6774 253.7520 0.6712
-0.2391 0.6712 240.5731
-187.3954 15.4893 4.5126
15.4893 -225.4389 -12.6911
4.5126 -12.6911 -82.8299

orbtensor 4 H
42.4976 0.5275 -1.8388
0.5275 23.2843 -0.0504
-1.8388 -0.0504 24.1076
-14.8418 -0.4814 0.4464
-0.4814 2.6979 0.0123
0.4464 0.0123 0.7841

orbtensor 5 C
253.5137 -0.0590 -0.7115

-0.0590 255.6577 -0.0186
-0.7115 -0.0186 240.5739
-230.9167 -1.3440 13.4587
-1.3440 -181.9225 0.3655
13.4587 0.3655 -82.8292

orbtensor 6 H
24.8089 5.2198 -0.5201
5.2198 40.9733 -1.7639
-0.5201 -1.7639 24.1074
1.3060 -4.7650 0.1258
-4.7650 -13.4492 0.4276
0.1258 0.4276 0.7839

orbtensor 7 C
255.4886 -0.5821 -0.2017
-0.5821 253.6841 -0.6801
-0.2017 -0.6801 240.5747
-185.7954 -13.3156 3.8075
-13.3156 -227.0126 12.9043
3.8075 12.9043 -82.8292

orbtensor 8 H
36.3616 -8.9736 1.5167
-8.9736 29.4210 -1.0396
1.5167 -1.0396 24.1077
-9.2389 8.1912 -0.3674
8.1912 -2.9038 0.2519
-0.3674 0.2519 0.7837

orbtensor 9 C
254.1987 1.0014 0.5846
1.0014 254.9740 -0.4004
0.5846 -0.4004 240.5752
-215.2385 22.8829 -11.0974
22.8829 -197.5450 7.6048
-11.0974 7.6048 -82.8299

orbtensor 10 H
35.3577 9.2995 1.4580
9.2995 30.4244 1.1218
1.4580 1.1218 24.1078
-8.3229 -8.4890 -0.3539
-8.4890 -3.8198 -0.2721
-0.3539 -0.2721 0.7839

orbtensor 11 C
254.3100 -1.0378 0.5622
-1.0378 254.8615 0.4344
0.5622 0.4344 240.5748
-212.6861 -23.7104 -10.6665
-23.7104 -200.1169 -8.2112
-10.6665 -8.2112 -82.8291

orbtensor 12 H
24.8091 5.2196 0.5204
5.2196 40.9734 1.7663
0.5204 1.7663 24.1083
1.3068 -4.7643 -0.1268
-4.7643 -13.4484 -0.4292
-0.1268 -0.4292 0.7822

orbtensor 13 C
255.4868 -0.5825 0.1977
-0.5825 253.6843 0.6812
0.1977 0.6812 240.5760
-185.7742 -13.3055 -3.8004

-13.3055 -226.9995 -12.9325
-3.8004 -12.9325 -82.8300

orbtensor 14 H
36.3614 -8.9731 -1.5208
-8.9731 29.4206 1.0420
-1.5208 1.0420 24.1073
-9.2395 8.1914 0.3711
8.1914 -2.9034 -0.2546
0.3711 -0.2546 0.7829

orbtensor 15 C
254.1995 1.0005 -0.5902
1.0005 254.9725 0.4030
-0.5902 0.4030 240.5729
-215.2726 22.8773 11.1353
22.8773 -197.5642 -7.6315
11.1353 -7.6315 -82.8323

orbtensor 16 H
35.3577 9.2994 -1.4602
9.2994 30.4245 -1.1232
-1.4602 -1.1232 24.1068
-8.3232 -8.4894 0.3558
-8.4894 -3.8197 0.2739
0.3558 0.2739 0.7828

orbtensor 17 C
254.3106 -1.0367 -0.5683
-1.0367 254.8609 -0.4344
-0.5683 -0.4344 240.5719
-212.7197 -23.7058 10.7000
-23.7058 -200.1417 8.2174
10.7000 8.2174 -82.8252

orbtensor 18 H
25.4291 -6.0732 0.6157
-6.0732 40.3533 -1.7334
0.6157 -1.7334 24.1074
0.7407 5.5441 -0.1497
5.5441 -12.8829 0.4203
-0.1497 0.4203 0.7821

orbtensor 19 C
255.4173 0.6774 0.2354
0.6774 253.7532 -0.6705
0.2354 -0.6705 240.5737
-187.3793 15.4785 -4.5037
15.4785 -225.4385 12.6914
-4.5037 12.6914 -82.8266

orbtensor 20 C
253.5134 -0.0591 0.7066
-0.0591 255.6566 0.0198
0.7066 0.0198 240.5759
-230.8759 -1.3405 -13.4552
-1.3405 -181.8820 -0.3756
-13.4552 -0.3756 -82.8268

orbtensor 21 H
42.4979 0.5271 1.8384
0.5271 23.2844 0.0502
1.8384 0.0502 24.1082
-14.8394 -0.4812 -0.4453
-0.4812 2.6985 -0.0122
-0.4453 -0.0122 0.7817

```

gtensor (ppt)
0.0418   -0.0000   0.0000
-0.0000   0.0418   0.0000
0.0000   0.0000  -0.1070
38.9868  -0.0005   0.0053
-0.0005  38.9871   0.0018
0.0053   0.0018   0.9469

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	40.5204	-3001.53703	32409.06822	218.86583	32627.93404	29626.39701
2	H	-3.6225	26.17657	259.35917	0.00273	259.36190	285.53847
3	C	3.6292	84.69300	-1033.15981	17.21968	-1015.94012	-931.24712
4	H	-3.6230	26.17657	259.39736	0.00298	259.40033	285.57690
5	C	3.6294	84.69230	-1033.20725	17.22274	-1015.98452	-931.29222
6	H	-3.6221	26.17677	259.33053	0.00282	259.33335	285.51012
7	C	3.6286	84.70340	-1032.98900	17.21391	-1015.77509	-931.07169
8	H	-3.6210	26.17710	259.25178	0.00246	259.25424	285.43134
9	C	3.6266	84.71150	-1032.41016	17.20617	-1015.20398	-930.49248
10	H	-3.6212	26.17703	259.27087	0.00250	259.27337	285.45041
11	C	3.6268	84.70473	-1032.46709	17.21000	-1015.25710	-930.55236
12	H	-3.6202	26.17713	259.19450	0.00275	259.19725	285.37438
13	C	3.6270	84.71447	-1032.51454	17.20647	-1015.30807	-930.59360
14	H	-3.6225	26.17643	259.35917	0.00317	259.36235	285.53878
15	C	3.6292	84.69193	-1033.15981	17.22357	-1015.93624	-931.24431
16	H	-3.6230	26.17630	259.39736	0.00319	259.40054	285.57684
17	C	3.6296	84.68560	-1033.27368	17.22661	-1016.04707	-931.36147
18	H	-3.6220	26.17657	259.32815	0.00257	259.33072	285.50729
19	C	3.6290	84.69993	-1033.08389	17.21512	-1015.86878	-931.16884
20	C	3.6272	84.72040	-1032.59045	17.20169	-1015.38876	-930.66836
21	H	-3.6200	26.17710	259.18257	0.00241	259.18497	285.36207
	ring 1H	-3.6217	26.17676	259.30714	0.00276	259.30990	285.48666
	ring 13C	3.6283	84.70173	-1032.88557	17.21459	-1015.67097	-930.96925

```

=====
3NiCp2-GTO-CAM-B3LYP
Temperature: 298
Spin: 1

```

```

atensor 2 H
-6.4118 -2.5348 -1.0632
-2.5348 -0.1833 2.9901
-1.0632 2.9901 -3.2496
-0.1309 -0.0620 -0.0409
-0.0620 0.0216 0.1151
-0.0409 0.1151 0.0108

```

```

atensor 3 C
1.1162 -0.3420 -1.0105
-0.3420 1.9569 2.8439
-1.0105 2.8439 13.3886
-0.2907 -0.0322 -0.0331
-0.0322 -0.2115 0.0930
-0.0331 0.0930 -0.0113

```

```

orbtensor 2 H
25.1769 -5.7170 -0.6062
-5.7170 39.2240 1.7051
-0.6062 1.7051 24.1833
2.2141 5.8086 0.4793

```

5.8086 -12.0582 -1.3483
0.4793 -1.3483 0.4796

orbtensor 3 C
250.6767 0.4292 -0.5891
0.4292 249.6209 1.6567
-0.5891 1.6567 238.4832
-178.8499 18.9184 6.2864
18.9184 -225.3255 -17.6797
6.2864 -17.6797 -75.5909

gtensor (ppt)
-0.0082 0.0000 0.0000
0.0000 -0.0082 0.0000
0.0000 0.0000 -0.1363
79.3761 -0.0007 0.0054
-0.0007 79.3764 0.0046
0.0054 0.0046 0.7856

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
ring 1H		-3.314	26.4066	240.4408	0.0698	240.5106	266.9172
ring 13C		5.316	86.3382	-1533.3776	29.6824	-1503.6951	-1417.3570

=====
3NiCp2-GTO-HF
Temperature: 288
Spin: 1

atensor 2 H
-5.1191 -2.1081 -1.3397
-2.1081 0.0642 3.7643
-1.3397 3.7643 -2.0270
-0.6759 -0.4022 -0.2012
-0.4022 0.3125 0.5656
-0.2012 0.5656 0.0012

atensor 3 C
2.8274 -0.4815 -1.0185
-0.4815 4.0076 2.8420
-1.0185 2.8420 9.0414
-0.8751 -0.1049 -0.1463
-0.1049 -0.6174 0.4111
-0.1463 0.4111 -0.0034

orbtensor 2 H
25.6837 -5.8577 -0.5493
-5.8577 40.0764 1.5451
-0.5493 1.5451 24.2291
15.6655 14.2255 4.5320
14.2255 -19.2865 -12.7452
4.5320 -12.7452 0.0941

orbtensor 3 C
253.0623 0.5698 -0.3659
0.5698 251.6608 1.0287
-0.3659 1.0287 237.3943
-111.6451 27.2088 18.2247
27.2088 -178.4773 -51.2549
18.2247 -51.2549 -59.8581

gtensor (ppt)
-0.0627 -0.0000 0.0000

```

-0.0000    -0.0627    0.0000
0.0000     0.0000   -0.1787
485.9655   -0.0001    0.0064
-0.0001   485.9666    0.0127
0.0064     0.0127    0.0314

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	-2.4814	28.82077	210.79470	2.69431	213.48902	242.30978
3	C	4.7935	130.71230	-1619.11196	99.85007	-1519.26189	-1388.54959
4	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
5	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
7	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
8	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
9	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
10	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
11	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
12	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
13	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
14	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
15	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
16	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
17	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
19	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
20	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
21	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
	ring 1H	-0.2481	2.88208	21.07947	0.26943	21.34890	24.23098
	ring 13C	0.4794	13.07123	-161.91120	9.98501	-151.92619	-138.85496

3NiCp2-GTO-LC-PBE0

Temperature: 298

Spin: 1

atensor 2 H

```

-6.1740 -2.4661 -1.1026
-2.4661 -0.1138 3.1003
-1.1026 3.1003 -3.0105
-0.1551 -0.0769 -0.0475
-0.0769 0.0338 0.1335
-0.0475 0.1335 0.0095

```

atensor 3 C

```

1.1118 -0.3679 -1.0499
-0.3679 2.0156 2.9505
-1.0499 2.9505 12.3211
-0.3233 -0.0368 -0.0370
-0.0368 -0.2330 0.1041
-0.0370 0.1041 -0.0097

```

orbtensor 2 H

```

24.6935 -6.0086 -0.7633
-6.0086 39.4572 2.1467
-0.7633 2.1467 23.7428
2.8997 6.2986 0.7906
6.2986 -12.5762 -2.2241
0.7906 -2.2241 0.4148

```

orbtensor 3 C

```

250.8441 0.5966 -1.0176

```

```

0.5966 249.3770 2.8614
-1.0176 2.8614 238.6045
-172.7544 18.7283 7.2878
18.7283 -218.7559 -20.4974
7.2878 -20.4974 -69.3429

```

```

gtensor (ppt)
-0.0178      0.0000      0.0000
0.0000     -0.0178      0.0000
0.0000      0.0000     -0.1445
97.3402     -0.0008      0.0089
-0.0008     97.3430      0.0069
0.0089      0.0069      0.5648

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
ring 1H		-3.137	26.2106	228.8665	0.1543	229.0207	255.2313
ring 13C		4.961	92.6575	-1439.1935	33.3178	-1405.8757	-1313.2183

```

=====
3NiCp2-GTO-PBE
Temperature: 298
Spin: 1

```

```

atensor 1 Ni
90.0009 -0.0004 0.0105
-0.0004 90.0009 0.0056
0.0105 0.0056 2.0703
-25.3644 0.0001 -0.0028
0.0001 -25.3645 -0.0014
-0.0028 -0.0014 -2.6669

```

```

atensor 2 H
-6.8769 -2.6557 -0.9171
-2.6557 -0.3507 2.5791
-0.9171 2.5791 -3.6462
-0.0800 -0.0304 -0.0263
-0.0304 -0.0053 0.0738
-0.0263 0.0738 0.0101

```

```

atensor 3 C
-0.7882 -0.2453 -0.9024
-0.2453 -0.1851 2.5385
-0.9024 2.5385 13.5819
-0.2186 -0.0309 -0.0265
-0.0309 -0.1428 0.0745
-0.0265 0.0745 -0.0110

```

```

atensor 4 H
0.5873 0.2309 -2.7362
0.2309 -7.8152 -0.0751
-2.7362 -0.0751 -3.6469
0.0054 0.0026 -0.0783
0.0026 -0.0907 -0.0022
-0.0783 -0.0022 0.0101

```

```

atensor 5 C
-0.0989 0.0215 -2.6938
0.0215 -0.8754 -0.0742
-2.6938 -0.0742 13.5823
-0.1319 0.0027 -0.0790
0.0027 -0.2295 -0.0022
-0.0790 -0.0022 -0.0110

```

atensor 6 H
-7.1467 2.2820 -0.7743
2.2820 -0.0786 -2.6257
-0.7743 -2.6257 -3.6457
-0.0831 0.0261 -0.0222
0.0261 -0.0022 -0.0752
-0.0222 -0.0752 0.0101

atensor 7 C
-0.8126 0.2108 -0.7619
0.2108 -0.1590 -2.5847
-0.7619 -2.5847 13.5766
-0.2218 0.0265 -0.0224
0.0265 -0.1397 -0.0758
-0.0224 -0.0758 -0.0110

atensor 8 H
-2.0945 -3.9229 2.2581
-3.9229 -5.1288 -1.5479
2.2581 -1.5479 -3.6442
-0.0252 -0.0450 0.0647
-0.0450 -0.0600 -0.0443
0.0647 -0.0443 0.0101

atensor 9 C
-0.3461 -0.3628 2.2224
-0.3628 -0.6267 -1.5233
2.2224 -1.5233 13.5712
-0.1631 -0.0457 0.0652
-0.0457 -0.1984 -0.0447
0.0652 -0.0447 -0.0110

atensor 10 H
-2.5335 4.0657 2.1698
4.0657 -4.6911 1.6693
2.1698 1.6693 -3.6445
-0.0303 0.0466 0.0621
0.0466 -0.0550 0.0478
0.0621 0.0478 0.0101

atensor 11 C
-0.3874 0.3758 2.1355
0.3758 -0.5871 1.6426
2.1355 1.6426 13.5738
-0.1682 0.0473 0.0626
0.0473 -0.1932 0.0482
0.0626 0.0482 -0.0110

atensor 12 H
-7.1445 2.2821 0.7745
2.2821 -0.0792 2.6264
0.7745 2.6264 -3.6436
-0.0831 0.0261 0.0222
0.0261 -0.0022 0.0752
0.0222 0.0752 0.0101

atensor 13 C
-0.8119 0.2112 0.7628
0.2112 -0.1593 2.5822
0.7628 2.5822 13.5720
-0.2219 0.0265 0.0224
0.0265 -0.1396 0.0758
0.0224 0.0758 -0.0110

atensor 14 H
-2.0971 -3.9238 -2.2583

-3.9238 -5.1314 1.5475
-2.2583 1.5475 -3.6459
-0.0253 -0.0449 -0.0646
-0.0449 -0.0600 0.0443
-0.0646 0.0443 0.0101

atensor 15 C
-0.3474 -0.3624 -2.2207
-0.3624 -0.6274 1.5215
-2.2207 1.5215 13.5830
-0.1631 -0.0455 -0.0652
-0.0455 -0.1984 0.0447
-0.0652 0.0447 -0.0110

atensor 16 H
-2.5361 4.0669 -2.1691
4.0669 -4.6929 -1.6691
-2.1691 -1.6691 -3.6468
-0.0303 0.0465 -0.0621
0.0465 -0.0550 -0.0478
-0.0621 -0.0478 0.0101

atensor 17 C
-0.3880 0.3758 -2.1338
0.3758 -0.5868 -1.6435
-2.1338 -1.6435 13.5853
-0.1682 0.0472 -0.0626
0.0472 -0.1932 -0.0482
-0.0626 -0.0482 -0.0110

atensor 18 H
-6.8752 -2.6559 0.9167
-2.6559 -0.3503 -2.5791
0.9167 -2.5791 -3.6456
-0.0800 -0.0304 0.0262
-0.0304 -0.0053 -0.0738
0.0262 -0.0738 0.0101

atensor 19 C
-0.7876 -0.2458 0.9030
-0.2458 -0.1845 -2.5387
0.9030 -2.5387 13.5777
-0.2186 -0.0308 0.0265
-0.0308 -0.1428 -0.0745
0.0265 -0.0745 -0.0110

atensor 20 C
-0.0959 0.0212 2.6929
0.0212 -0.8729 0.0726
2.6929 0.0726 13.5695
-0.1318 0.0027 0.0790
0.0027 -0.2296 0.0021
0.0790 0.0021 -0.0110

atensor 21 H
0.5883 0.2304 2.7369
0.2304 -7.8103 0.0747
2.7369 0.0747 -3.6435
0.0055 0.0026 0.0784
0.0026 -0.0908 0.0021
0.0784 0.0021 0.0101

orbtensor 1 Ni
2271.1358 -0.0002 0.0042
-0.0002 2271.1359 0.0000
0.0042 0.0000 2274.7087
-7699.7855 0.0401 -0.1200

0.0401 -7699.7997 -0.3955
-0.1200 -0.3955 -643.0200

orbtensor 2 H
25.3153 -5.8486 -0.5893
-5.8486 39.6856 1.6574
-0.5893 1.6574 24.1722
0.8270 5.3447 0.1343
5.3447 -12.3050 -0.3784
0.1343 -0.3784 0.6244

orbtensor 3 C
251.5222 0.2807 -0.6549
0.2807 250.8303 1.8409
-0.6549 1.8409 238.7556
-183.3580 15.9224 4.9965
15.9224 -222.4649 -14.0520
4.9965 -14.0520 -80.7988

orbtensor 4 H
41.7517 0.5079 -1.7572
0.5079 23.2499 -0.0482
-1.7572 -0.0482 24.1723
-14.1930 -0.4640 0.4004
-0.4640 2.7144 0.0111
0.4004 0.0111 0.6245

orbtensor 5 C
250.7329 -0.0247 -1.9521
-0.0247 251.6221 -0.0527
-1.9521 -0.0527 238.7563
-228.0940 -1.3811 14.9032
-1.3811 -177.7305 0.4053
14.9032 0.4053 -80.7976

orbtensor 6 H
24.7181 5.0265 -0.4970
5.0265 40.2838 -1.6856
-0.4970 -1.6856 24.1720
1.3726 -4.5932 0.1127
-4.5932 -12.8507 0.3837
0.1127 0.3837 0.6246

orbtensor 7 C
251.5530 -0.2411 -0.5526
-0.2411 250.8037 -1.8706
-0.5526 -1.8706 238.7574
-181.7124 -13.6885 4.2160
-13.6885 -224.0828 14.2897
4.2160 14.2897 -80.7982

orbtensor 8 H
35.8429 -8.6412 1.4494
-8.6412 29.1593 -0.9935
1.4494 -0.9935 24.1724
-8.7921 7.8959 -0.3297
7.8959 -2.6853 0.2260
-0.3297 0.2260 0.6246

orbtensor 9 C
251.0169 0.4155 1.6084
0.4155 251.3388 -1.1022
1.6084 -1.1022 238.7580
-211.9803 23.5238 -12.2885
23.5238 -193.7908 8.4213
-12.2885 8.4213 -80.7993

orbtensor 10 H
34.8761 8.9551 1.3934
8.9551 30.1254 1.0721
1.3934 1.0721 24.1724
-7.9090 -8.1830 -0.3176
-8.1830 -3.5682 -0.2440
-0.3176 -0.2440 0.6246

orbtensor 11 C
251.0620 -0.4306 1.5461
-0.4306 251.2918 1.1911
1.5461 1.1911 238.7575
-209.3537 -24.3737 -11.8121
-24.3737 -196.4337 -9.0923
-11.8121 -9.0923 -80.7979

orbtensor 12 H
24.7183 5.0262 0.4973
5.0262 40.2840 1.6879
0.4973 1.6879 24.1730
1.3729 -4.5926 -0.1141
-4.5926 -12.8506 -0.3857
-0.1141 -0.3857 0.6247

orbtensor 13 C
251.5508 -0.2419 0.5490
-0.2419 250.8037 1.8718
0.5490 1.8718 238.7588
-181.6947 -13.6780 -4.2087
-13.6780 -224.0743 -14.3170
-4.2087 -14.3170 -80.8015

orbtensor 14 H
35.8428 -8.6408 -1.4534
-8.6408 29.1591 0.9958
-1.4534 0.9958 24.1719
-8.7933 7.8962 0.3335
7.8962 -2.6856 -0.2288
0.3335 -0.2288 0.6250

orbtensor 15 C
251.0180 0.4149 -1.6140
0.4149 251.3375 1.1046
-1.6140 1.1046 238.7555
-212.0168 23.5172 12.3262
23.5172 -193.8132 -8.4475
12.3262 -8.4475 -80.8029

orbtensor 16 H
34.8763 8.9549 -1.3955
8.9549 30.1258 -1.0734
-1.3955 -1.0734 24.1715
-7.9102 -8.1835 0.3196
-8.1835 -3.5690 0.2462
0.3196 0.2462 0.6251

orbtensor 17 C
251.0636 -0.4296 -1.5520
-0.4296 251.2917 -1.1915
-1.5520 -1.1915 238.7543
-209.3944 -24.3700 11.8433
-24.3700 -196.4633 9.0973
11.8433 9.0973 -80.7959

orbtensor 18 H
25.3154 -5.8482 0.5884
-5.8482 39.6869 -1.6564

0.5884 -1.6564 24.1721
 0.8271 5.3443 -0.1347
 5.3443 -12.3054 0.3777
 -0.1347 0.3777 0.6248

orbtensor 19 C
 251.5216 0.2812 0.6515
 0.2812 250.8326 -1.8402
 0.6515 -1.8402 238.7560
 -183.3422 15.9126 -4.9872
 15.9126 -222.4688 14.0520
 -4.9872 14.0520 -80.7975

orbtensor 20 C
 250.7325 -0.0249 1.9478
 -0.0249 251.6212 0.0537
 1.9478 0.0537 238.7587
 -228.0616 -1.3784 -14.8975
 -1.3784 -177.6937 -0.4149
 -14.8975 -0.4149 -80.7989

orbtensor 21 H
 41.7519 0.5076 1.7568
 0.5076 23.2501 0.0480
 1.7568 0.0480 24.1728
 -14.1915 -0.4639 -0.4002
 -0.4639 2.7143 -0.0109
 -0.4002 -0.0109 0.6246

gtensor (ppt)
 0.0429 -0.0000 0.0000
 -0.0000 0.0429 0.0000
 0.0000 0.0000 -0.1083
 40.1456 -0.0005 0.0051
 -0.0005 40.1459 0.0025
 0.0051 0.0025 0.9899

averaging
 1H Average:2,4,6,8,10,12,14,16,18,21
 13C Average:3,5,7,9,11,13,15,17,19,20

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	42.8921	-3075.20827	34319.31555	224.65604	34543.97159	31468.76333
2	H	-3.6497	26.10650	261.40802	0.00619	261.41420	287.52070
3	C	4.0787	84.82880	-1161.57274	17.45268	-1144.12006	-1059.29126
4	H	-3.6500	26.10660	261.43189	0.00646	261.43836	287.54496
5	C	4.0785	84.82973	-1161.51578	17.45532	-1144.06046	-1059.23073
6	H	-3.6487	26.10680	261.34117	0.00634	261.34751	287.45431
7	C	4.0775	84.84023	-1161.22150	17.44639	-1143.77511	-1058.93487
8	H	-3.6475	26.10727	261.25522	0.00599	261.26120	287.36847
9	C	4.0753	84.84777	-1160.59497	17.43877	-1143.15620	-1058.30844
10	H	-3.6481	26.10710	261.29580	0.00602	261.30182	287.40892
11	C	4.0756	84.84200	-1160.68990	17.44225	-1143.24765	-1058.40565
12	H	-3.6475	26.10743	261.25283	0.00623	261.25906	287.36650
13	C	4.0761	84.84760	-1160.82280	17.43852	-1143.38428	-1058.53668
14	H	-3.6499	26.10663	261.42234	0.00665	261.42899	287.53562
15	C	4.0786	84.82603	-1161.52527	17.45590	-1144.06937	-1059.24334
16	H	-3.6503	26.10650	261.45577	0.00673	261.46249	287.56899
17	C	4.0794	84.81867	-1161.75310	17.45942	-1144.29368	-1059.47502
18	H	-3.6488	26.10697	261.34355	0.00613	261.34969	287.45665
19	C	4.0777	84.83390	-1161.28795	17.44713	-1143.84082	-1059.00692
20	C	4.0761	84.85273	-1160.82280	17.43358	-1143.38922	-1058.53649
21	H	-3.6469	26.10740	261.20985	0.00592	261.21577	287.32317

ring 1H	-3.6487	26.10692	261.34164	0.00627	261.34791	287.45483
ring 13C	4.0774	84.83675	-1161.18068	17.44700	-1143.73368	-1058.89694

=====
 3NiCp2-GTO-PBE0
 Temperature: 298
 Spin: 1

atensor 2 H
 -6.4314 -2.5007 -1.0553
 -2.5007 -0.2865 2.9678
 -1.0553 2.9678 -3.2124
 -0.1373 -0.0649 -0.0426
 -0.0649 0.0223 0.1199
 -0.0426 0.1199 0.0103

atensor 3 C
 1.0150 -0.3405 -1.0050
 -0.3405 1.8518 2.8274
 -1.0050 2.8274 12.8568
 -0.2941 -0.0338 -0.0355
 -0.0338 -0.2109 0.0997
 -0.0355 0.0997 -0.0110

orbtensor 2 H
 25.2141 -5.8748 -0.6067
 -5.8748 39.6489 1.7064
 -0.6067 1.7064 24.0464
 2.1613 5.9937 0.5111
 5.9937 -12.5656 -1.4377
 0.5111 -1.4377 0.4853

orbtensor 3 C
 251.4679 0.3363 -0.7232
 0.3363 250.6400 2.0331
 -0.7232 2.0331 238.5496
 -175.5992 17.5830 6.3522
 17.5830 -218.7915 -17.8647
 6.3522 -17.8647 -74.2763

gtensor (ppt)
 0.0005 0.0000 0.0000
 0.0000 0.0005 0.0000
 0.0000 0.0000 -0.1356
 82.9446 -0.0014 0.0075
 -0.0014 82.9459 0.0096
 0.0075 0.0096 0.7936

averaging
 1H Average:2,4,6,8,10,12,14,16,18,21
 13C Average:3,5,7,9,11,13,15,17,19,20

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	-3.3450	26.33013	242.94261	0.13770	243.08031	269.41044
3	C	5.0692	90.66350	-1463.86959	29.93142	-1433.93817	-1343.27467
4	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
5	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
7	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
8	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
9	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
10	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
11	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000

12	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
13	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
14	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
15	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
16	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
17	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
19	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
20	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
21	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
ring 1H		-0.3345	2.63301	24.29426	0.01377	24.30803	26.94104
ring 13C		0.5069	9.06635	-146.38696	2.99314	-143.39382	-134.32747

=====
4VCp2-STO-B3LYP-No-ZFS

Temperature: 298

Spin: 1.5

atensor 1 V

6.789 0.000 0.000
0.000 6.789 0.004
0.000 0.004 -53.784
-10.041 0.000 0.000
0.000 -10.041 0.000
0.000 0.000 -4.532

atensor 2 H

0.679 -1.424 -1.291
-1.424 4.177 3.631
-1.291 3.631 3.917
0.019 0.007 0.011
0.007 0.002 -0.030
0.004 -0.010 -0.002

atensor 3 C

-1.675 -0.258 -0.600
-0.258 -1.041 1.688
-0.600 1.687 0.721
0.051 0.007 0.009
0.007 0.033 -0.026
0.007 -0.020 0.000

atensor 4 H

4.680 0.124 -3.852
0.124 0.176 -0.106
-3.852 -0.106 3.916
0.000 -0.001 0.031
-0.001 0.022 0.001
0.011 0.000 -0.002

atensor 5 C

-0.949 0.022 -1.791
0.022 -1.766 -0.049
-1.790 -0.049 0.721
0.031 -0.001 0.027
-0.001 0.053 0.001
0.022 0.001 0.000

atensor 6 H

0.533 1.224 -1.090
1.224 4.323 -3.696
-1.090 -3.696 3.916
0.020 -0.006 0.009
-0.006 0.002 0.030
0.003 0.010 -0.002

atensor 7 C
-1.701 0.222 -0.507
0.222 -1.014 -1.718
-0.507 -1.718 0.722
0.051 -0.006 0.008
-0.006 0.032 0.026
0.006 0.021 0.000

atensor 8 H
3.241 -2.104 3.178
-2.104 1.614 -2.179
3.178 -2.179 3.917
0.007 0.010 -0.026
0.010 0.015 0.018
-0.009 0.006 -0.002

atensor 9 C
-1.210 -0.381 1.477
-0.381 -1.505 -1.013
1.477 -1.013 0.722
0.038 0.011 -0.022
0.011 0.046 0.015
-0.018 0.012 0.000

atensor 10 H
3.006 2.180 3.054
2.180 1.849 2.350
3.054 2.350 3.917
0.008 -0.011 -0.025
-0.011 0.014 -0.019
-0.009 -0.007 -0.002

atensor 11 C
-1.254 0.395 1.420
0.395 -1.463 1.092
1.419 1.092 0.721
0.039 -0.011 -0.022
-0.011 0.045 -0.017
-0.017 -0.013 0.000

atensor 12 H
0.533 1.224 1.090
1.224 4.322 3.696
1.090 3.696 3.917
0.020 -0.006 -0.009
-0.006 0.002 -0.030
-0.003 -0.010 -0.002

atensor 13 C
-1.701 0.222 0.507
0.222 -1.015 1.718
0.507 1.718 0.721
0.051 -0.006 -0.008
-0.006 0.032 -0.026
-0.006 -0.021 0.000

atensor 14 H
3.241 -2.103 -3.179
-2.103 1.614 2.179
-3.179 2.178 3.917
0.007 0.010 0.026
0.010 0.015 -0.018
0.009 -0.006 -0.002

atensor 15 C
-1.211 -0.381 -1.477
-0.381 -1.506 1.012

-1.477 1.012 0.722
0.038 0.011 0.022
0.011 0.046 -0.015
0.018 -0.012 0.000

atensor 16 H
3.006 2.180 -3.054
2.180 1.849 -2.350
-3.054 -2.350 3.916
0.008 -0.011 0.025
-0.011 0.014 0.019
0.009 0.007 -0.002

atensor 17 C
-1.253 0.395 -1.420
0.395 -1.463 -1.092
-1.420 -1.092 0.721
0.039 -0.011 0.022
-0.011 0.045 0.017
0.017 0.013 0.000

atensor 18 H
0.679 -1.424 1.291
-1.424 4.178 -3.631
1.291 -3.631 3.916
0.019 0.007 -0.011
0.007 0.002 0.030
-0.004 0.010 -0.002

atensor 19 C
-1.675 -0.258 0.600
-0.258 -1.041 -1.688
0.600 -1.688 0.721
0.051 0.007 -0.009
0.007 0.033 0.026
-0.007 0.020 0.000

atensor 20 C
-0.950 0.022 1.790
0.022 -1.766 0.049
1.790 0.049 0.721
0.031 -0.001 -0.027
-0.001 0.053 -0.001
-0.022 -0.001 0.000

atensor 21 H
4.680 0.123 3.852
0.123 0.176 0.105
3.852 0.105 3.916
0.000 -0.001 -0.031
-0.001 0.022 -0.001
-0.011 0.000 -0.002

orbtensor 1 V
-3695.667 0.005 -0.023
0.005 -3695.668 -0.184
-0.023 -0.184 -277.304
1694.686 0.000 0.000
0.000 1694.686 -0.001
0.000 -0.001 1713.093

orbtensor 2 H
-1.769 4.331 0.631
4.331 -12.410 -1.776
0.631 -1.776 -0.272
28.220 -4.785 -0.729
-4.785 39.978 2.052

```

-0.729    2.052    25.424

orbtensor 3 C
-189.494   18.310    7.878
18.310  -234.479  -22.174
7.878  -22.174  -71.558
255.949    2.282    -1.301
2.282  250.340    3.663
-1.301    3.663   232.449

orbtensor 4 H
-13.939   -0.376    1.884
-0.376   -0.240    0.052
1.884    0.052   -0.271
41.668    0.416   -2.176
0.416   26.530   -0.060
-2.176   -0.060   25.424

orbtensor 5 C
-240.947   -1.591   23.515
-1.591 -183.027    0.642
23.515    0.642  -71.556
249.535   -0.198   -3.885
-0.198  256.755   -0.106
-3.885   -0.106  232.449

orbtensor 6 H
-1.327   -3.722    0.533
-3.722  -12.852    1.808
0.533    1.808   -0.271
27.731    4.113   -0.616
4.113   40.467   -2.088
-0.616   -2.088   25.424

orbtensor 7 C
-187.624  -15.737    6.650
-15.737 -236.350   22.566
6.650   22.566  -71.556
256.181   -1.962   -1.098
-1.962  250.107   -3.728
-1.098   -3.728  232.448

orbtensor 8 H
-9.564    6.398   -1.555
6.398   -4.615    1.066
-1.555    1.066   -0.271
36.833   -7.070    1.796
-7.070   31.365   -1.231
1.796   -1.231   25.424

orbtensor 9 C
-222.445   27.051  -19.415
27.051 -201.525   13.302
-19.415   13.302  -71.558
251.840    3.372    3.207
3.372  254.448   -2.197
3.207   -2.197  232.449

orbtensor 10 H
-8.848   -6.630   -1.495
-6.630   -5.330   -1.150
-1.495   -1.150   -0.272
36.043    7.327    1.727
7.327   32.155    1.328
1.727    1.328   25.424

orbtensor 11 C

```



```
-219.420  -28.032  -18.658
-28.032  -204.549  -14.352
-18.658  -14.352  -71.560
252.217   -3.495   3.082
-3.495  254.071   2.370
3.082    2.370  232.449
```

```
orbtensor 12 H
-1.327   -3.722   -0.533
-3.722  -12.852   -1.809
-0.533   -1.809   -0.272
27.731   4.113    0.616
4.113   40.467    2.090
0.616    2.090   25.424
```

```
orbtensor 13 C
-187.624  -15.736   -6.652
-15.736  -236.346  -22.582
-6.652  -22.582  -71.560
256.182  -1.962    1.098
-1.962  250.107    3.730
1.098    3.730  232.449
```

```
orbtensor 14 H
-9.564    6.398    1.555
6.398   -4.615   -1.066
1.555   -1.066   -0.272
36.833   -7.070   -1.797
-7.070   31.365    1.232
-1.797    1.232   25.424
```

```
orbtensor 15 C
-222.446   27.049   19.414
27.049  -201.522  -13.313
19.414  -13.313  -71.559
251.840    3.372   -3.206
3.372  254.448    2.199
-3.206    2.199  232.449
```

```
orbtensor 16 H
-8.848   -6.631    1.494
-6.631   -5.331    1.149
1.494    1.149   -0.271
36.043    7.327   -1.726
7.327   32.156   -1.327
-1.726   -1.327   25.424
```

```
orbtensor 17 C
-219.420  -28.035   18.650
-28.035  -204.552   14.336
18.650   14.336  -71.556
252.217   -3.494   -3.081
-3.494  254.072   -2.368
-3.081   -2.368  232.448
```

```
orbtensor 18 H
-1.769    4.331   -0.631
4.331  -12.410    1.775
-0.631    1.775   -0.271
28.220   -4.785    0.729
-4.785   39.978   -2.050
0.729   -2.050   25.424
```

```
orbtensor 19 C
-189.494   18.310   -7.877
18.310  -234.483   22.156
-7.877   22.156  -71.554
```

255.949 2.282 1.302
 2.282 250.341 -3.661
 1.302 -3.661 232.448

orbtensor 20 C
 -240.948 -1.588 -23.516
 -1.588 -183.027 -0.654
 -23.516 -0.654 -71.556
 249.534 -0.198 3.885
 -0.198 256.755 0.109
 3.885 0.109 232.448

orbtensor 21 H
 -13.939 -0.376 -1.884
 -0.376 -0.240 -0.052
 -1.884 -0.052 -0.271
 41.668 0.416 2.176
 0.416 26.530 0.060
 2.176 0.060 25.424

gtensor (ppt)
 -0.146 0.000 0.000
 0.000 -0.146 0.000
 0.000 0.000 -0.134
 -11.237 0.000 0.000
 0.000 -11.237 -0.001
 0.000 -0.001 -1.013

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-21.6067	-855.39133	10827.64581	31.47247	10859.11828	10003.72694
2	H	2.9307	26.39033	-386.78100	-0.22209	-387.00310	-360.61276
3	C	-0.6370	81.06900	334.26820	-1.21888	333.04933	414.11833
4	H	2.9307	26.39067	-386.78100	-0.22203	-387.00304	-360.61237
5	C	-0.6367	81.06967	334.09329	-1.21888	332.87441	413.94408
6	H	2.9307	26.39067	-386.78100	-0.22219	-387.00319	-360.61253
7	C	-0.6367	81.06867	334.09329	-1.22006	332.87322	413.94189
8	H	2.9307	26.39067	-386.78100	-0.22235	-387.00335	-360.61269
9	C	-0.6363	81.06967	333.91837	-1.21964	332.69873	413.76839
10	H	2.9307	26.39067	-386.78100	-0.22215	-387.00315	-360.61249
11	C	-0.6373	81.06933	334.44312	-1.21928	333.22384	414.29318
12	H	2.9307	26.39033	-386.78100	-0.22209	-387.00310	-360.61276
13	C	-0.6373	81.06933	334.44312	-1.21917	333.22395	414.29329
14	H	2.9307	26.39033	-386.78100	-0.22216	-387.00316	-360.61283
15	C	-0.6370	81.07000	334.26820	-1.21989	333.04831	414.11831
16	H	2.9303	26.39100	-386.73701	-0.22221	-386.95922	-360.56822
17	C	-0.6370	81.06967	334.26820	-1.21936	333.04885	414.11851
18	H	2.9307	26.39067	-386.78100	-0.22219	-387.00319	-360.61252
19	C	-0.6370	81.06900	334.26820	-1.21946	333.04875	414.11775
20	C	-0.6370	81.06867	334.26820	-1.21916	333.04905	414.11771
21	H	2.9307	26.39067	-386.78100	-0.22202	-387.00303	-360.61236
13C Average		-0.6369	81.06930	334.23322	-1.21938	333.01384	414.08314
1H Average		2.9306	26.39060	-386.77660	-0.22215	-386.99875	-360.60815

=====
 4VCp2-STO-B3LYP-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 V

6.789 0.000 0.000
0.000 6.789 0.004
0.000 0.004 -53.784
-10.041 0.000 0.000
0.000 -10.041 0.000
0.000 0.000 -4.532

atensor 2 H
0.679 -1.424 -1.291
-1.424 4.177 3.631
-1.291 3.631 3.917
0.019 0.007 0.011
0.007 0.002 -0.030
0.004 -0.010 -0.002

atensor 3 C
-1.675 -0.258 -0.600
-0.258 -1.041 1.688
-0.600 1.687 0.721
0.051 0.007 0.009
0.007 0.033 -0.026
0.007 -0.020 0.000

atensor 4 H
4.680 0.124 -3.852
0.124 0.176 -0.106
-3.852 -0.106 3.916
0.000 -0.001 0.031
-0.001 0.022 0.001
0.011 0.000 -0.002

atensor 5 C
-0.949 0.022 -1.791
0.022 -1.766 -0.049
-1.790 -0.049 0.721
0.031 -0.001 0.027
-0.001 0.053 0.001
0.022 0.001 0.000

atensor 6 H
0.533 1.224 -1.090
1.224 4.323 -3.696
-1.090 -3.696 3.916
0.020 -0.006 0.009
-0.006 0.002 0.030
0.003 0.010 -0.002

atensor 7 C
-1.701 0.222 -0.507
0.222 -1.014 -1.718
-0.507 -1.718 0.722
0.051 -0.006 0.008
-0.006 0.032 0.026
0.006 0.021 0.000

atensor 8 H
3.241 -2.104 3.178
-2.104 1.614 -2.179
3.178 -2.179 3.917
0.007 0.010 -0.026
0.010 0.015 0.018
-0.009 0.006 -0.002

atensor 9 C
-1.210 -0.381 1.477
-0.381 -1.505 -1.013
1.477 -1.013 0.722

0.038 0.011 -0.022
0.011 0.046 0.015
-0.018 0.012 0.000

atensor 10 H
3.006 2.180 3.054
2.180 1.849 2.350
3.054 2.350 3.917
0.008 -0.011 -0.025
-0.011 0.014 -0.019
-0.009 -0.007 -0.002

atensor 11 C
-1.254 0.395 1.420
0.395 -1.463 1.092
1.419 1.092 0.721
0.039 -0.011 -0.022
-0.011 0.045 -0.017
-0.017 -0.013 0.000

atensor 12 H
0.533 1.224 1.090
1.224 4.322 3.696
1.090 3.696 3.917
0.020 -0.006 -0.009
-0.006 0.002 -0.030
-0.003 -0.010 -0.002

atensor 13 C
-1.701 0.222 0.507
0.222 -1.015 1.718
0.507 1.718 0.721
0.051 -0.006 -0.008
-0.006 0.032 -0.026
-0.006 -0.021 0.000

atensor 14 H
3.241 -2.103 -3.179
-2.103 1.614 2.179
-3.179 2.178 3.917
0.007 0.010 0.026
0.010 0.015 -0.018
0.009 -0.006 -0.002

atensor 15 C
-1.211 -0.381 -1.477
-0.381 -1.506 1.012
-1.477 1.012 0.722
0.038 0.011 0.022
0.011 0.046 -0.015
0.018 -0.012 0.000

atensor 16 H
3.006 2.180 -3.054
2.180 1.849 -2.350
-3.054 -2.350 3.916
0.008 -0.011 0.025
-0.011 0.014 0.019
0.009 0.007 -0.002

atensor 17 C
-1.253 0.395 -1.420
0.395 -1.463 -1.092
-1.420 -1.092 0.721
0.039 -0.011 0.022
-0.011 0.045 0.017
0.017 0.013 0.000

atensor 18 H
0.679 -1.424 1.291
-1.424 4.178 -3.631
1.291 -3.631 3.916
0.019 0.007 -0.011
0.007 0.002 0.030
-0.004 0.010 -0.002

atensor 19 C
-1.675 -0.258 0.600
-0.258 -1.041 -1.688
0.600 -1.688 0.721
0.051 0.007 -0.009
0.007 0.033 0.026
-0.007 0.020 0.000

atensor 20 C
-0.950 0.022 1.790
0.022 -1.766 0.049
1.790 0.049 0.721
0.031 -0.001 -0.027
-0.001 0.053 -0.001
-0.022 -0.001 0.000

atensor 21 H
4.680 0.123 3.852
0.123 0.176 0.105
3.852 0.105 3.916
0.000 -0.001 -0.031
-0.001 0.022 -0.001
-0.011 0.000 -0.002

orbtensor 1 V
-3695.667 0.005 -0.023
0.005 -3695.668 -0.184
-0.023 -0.184 -277.304
1694.686 0.000 0.000
0.000 1694.686 -0.001
0.000 -0.001 1713.093

orbtensor 2 H
-1.769 4.331 0.631
4.331 -12.410 -1.776
0.631 -1.776 -0.272
28.220 -4.785 -0.729
-4.785 39.978 2.052
-0.729 2.052 25.424

orbtensor 3 C
-189.494 18.310 7.878
18.310 -234.479 -22.174
7.878 -22.174 -71.558
255.949 2.282 -1.301
2.282 250.340 3.663
-1.301 3.663 232.449

orbtensor 4 H
-13.939 -0.376 1.884
-0.376 -0.240 0.052
1.884 0.052 -0.271
41.668 0.416 -2.176
0.416 26.530 -0.060
-2.176 -0.060 25.424

orbtensor 5 C
-240.947 -1.591 23.515

-1.591	-183.027	0.642
23.515	0.642	-71.556
249.535	-0.198	-3.885
-0.198	256.755	-0.106
-3.885	-0.106	232.449

orbtensor 6 H

-1.327	-3.722	0.533
-3.722	-12.852	1.808
0.533	1.808	-0.271
27.731	4.113	-0.616
4.113	40.467	-2.088
-0.616	-2.088	25.424

orbtensor 7 C

-187.624	-15.737	6.650
-15.737	-236.350	22.566
6.650	22.566	-71.556
256.181	-1.962	-1.098
-1.962	250.107	-3.728
-1.098	-3.728	232.448

orbtensor 8 H

-9.564	6.398	-1.555
6.398	-4.615	1.066
-1.555	1.066	-0.271
36.833	-7.070	1.796
-7.070	31.365	-1.231
1.796	-1.231	25.424

orbtensor 9 C

-222.445	27.051	-19.415
27.051	-201.525	13.302
-19.415	13.302	-71.558
251.840	3.372	3.207
3.372	254.448	-2.197
3.207	-2.197	232.449

orbtensor 10 H

-8.848	-6.630	-1.495
-6.630	-5.330	-1.150
-1.495	-1.150	-0.272
36.043	7.327	1.727
7.327	32.155	1.328
1.727	1.328	25.424

orbtensor 11 C

-219.420	-28.032	-18.658
-28.032	-204.549	-14.352
-18.658	-14.352	-71.560
252.217	-3.495	3.082
-3.495	254.071	2.370
3.082	2.370	232.449

orbtensor 12 H

-1.327	-3.722	-0.533
-3.722	-12.852	-1.809
-0.533	-1.809	-0.272
27.731	4.113	0.616
4.113	40.467	2.090
0.616	2.090	25.424

orbtensor 13 C

-187.624	-15.736	-6.652
-15.736	-236.346	-22.582
-6.652	-22.582	-71.560
256.182	-1.962	1.098

-1.962 250.107 3.730
1.098 3.730 232.449

orbtensor 14 H
-9.564 6.398 1.555
6.398 -4.615 -1.066
1.555 -1.066 -0.272
36.833 -7.070 -1.797
-7.070 31.365 1.232
-1.797 1.232 25.424

orbtensor 15 C
-222.446 27.049 19.414
27.049 -201.522 -13.313
19.414 -13.313 -71.559
251.840 3.372 -3.206
3.372 254.448 2.199
-3.206 2.199 232.449

orbtensor 16 H
-8.848 -6.631 1.494
-6.631 -5.331 1.149
1.494 1.149 -0.271
36.043 7.327 -1.726
7.327 32.156 -1.327
-1.726 -1.327 25.424

orbtensor 17 C
-219.420 -28.035 18.650
-28.035 -204.552 14.336
18.650 14.336 -71.556
252.217 -3.494 -3.081
-3.494 254.072 -2.368
-3.081 -2.368 232.448

orbtensor 18 H
-1.769 4.331 -0.631
4.331 -12.410 1.775
-0.631 1.775 -0.271
28.220 -4.785 0.729
-4.785 39.978 -2.050
0.729 -2.050 25.424

orbtensor 19 C
-189.494 18.310 -7.877
18.310 -234.483 22.156
-7.877 22.156 -71.554
255.949 2.282 1.302
2.282 250.341 -3.661
1.302 -3.661 232.448

orbtensor 20 C
-240.948 -1.588 -23.516
-1.588 -183.027 -0.654
-23.516 -0.654 -71.556
249.534 -0.198 3.885
-0.198 256.755 0.109
3.885 0.109 232.448

orbtensor 21 H
-13.939 -0.376 -1.884
-0.376 -0.240 -0.052
-1.884 -0.052 -0.271
41.668 0.416 2.176
0.416 26.530 0.060
2.176 0.060 25.424

```

gtensor (ppt)
-0.146    0.000    0.000
0.000   -0.146    0.000
0.000    0.000   -0.134
-11.237    0.000    0.000
0.000   -11.237   -0.001
0.000   -0.001   -1.013

```

```

zfstensor (cm-1)
-1.119985    0.000013   -0.000016
 0.000013   -1.120151   -0.000097
-0.000016   -0.000097    1.385561

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-21.6067	-855.39133	10827.25563	-57.51409	10769.74154	9914.35021
2	H	2.9307	26.39033	-386.76707	0.40606	-386.36100	-359.97067
3	C	-0.6370	81.06900	334.25616	2.22788	336.48404	417.55304
4	H	2.9307	26.39067	-386.76707	0.40587	-386.36120	-359.97053
5	C	-0.6367	81.06967	334.08125	2.22754	336.30878	417.37845
6	H	2.9307	26.39067	-386.76707	0.40570	-386.36137	-359.97070
7	C	-0.6367	81.06867	334.08125	2.22905	336.31030	417.37897
8	H	2.9307	26.39067	-386.76707	0.40616	-386.36090	-359.97024
9	C	-0.6363	81.06967	333.90634	2.22849	336.13483	417.20450
10	H	2.9307	26.39067	-386.76707	0.40616	-386.36091	-359.97024
11	C	-0.6373	81.06933	334.43107	2.22846	336.65953	417.72887
12	H	2.9307	26.39033	-386.76707	0.40606	-386.36101	-359.97068
13	C	-0.6373	81.06933	334.43107	2.22840	336.65947	417.72881
14	H	2.9307	26.39033	-386.76707	0.40619	-386.36088	-359.97054
15	C	-0.6370	81.07000	334.25616	2.22964	336.48580	417.55580
16	H	2.9303	26.39100	-386.72308	0.40596	-386.31712	-359.92612
17	C	-0.6370	81.06967	334.25616	2.22805	336.48421	417.55388
18	H	2.9307	26.39067	-386.76707	0.40567	-386.36140	-359.97073
19	C	-0.6370	81.06900	334.25616	2.22792	336.48407	417.55307
20	C	-0.6370	81.06867	334.25616	2.22797	336.48413	417.55279
21	H	2.9307	26.39067	-386.76707	0.40581	-386.36126	-359.97059
13C Average		-0.6369	81.06930	334.22118	2.22834	336.44952	417.51882
1H Average		2.9306	26.39060	-386.76267	0.40596	-386.35670	-359.96610

```

=====
4VCp2-STO-BHLYP-No-ZFS
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
-48.726 0.000 0.000
0.000 -48.727 0.004
0.000 0.004 -110.036
-12.485 0.000 0.000
0.000 -12.485 0.000
0.000 0.000 -3.736

```

```

atensor 2 H
0.427 -1.422 -1.320
-1.422 3.919 3.713
-1.320 3.713 3.607
0.027 0.012 0.016
0.012 -0.002 -0.044
0.003 -0.008 -0.001

```


atensor 3 C
-1.788 -0.273 -0.608
-0.273 -1.117 1.711
-0.608 1.711 0.442
0.057 0.008 0.012
0.008 0.038 -0.035
0.007 -0.019 0.001

atensor 4 H
4.421 0.124 -3.940
0.124 -0.076 -0.108
-3.940 -0.108 3.607
-0.006 -0.001 0.046
-0.001 0.031 0.001
0.009 0.000 -0.001

atensor 5 C
-1.019 0.024 -1.816
0.024 -1.883 -0.050
-1.816 -0.050 0.443
0.036 -0.001 0.037
-0.001 0.059 0.001
0.020 0.001 0.001

atensor 6 H
0.281 1.222 -1.115
1.222 4.064 -3.780
-1.115 -3.780 3.607
0.028 -0.010 0.013
-0.010 -0.003 0.044
0.002 0.008 -0.001

atensor 7 C
-1.814 0.235 -0.514
0.235 -1.087 -1.742
-0.514 -1.742 0.444
0.058 -0.007 0.011
-0.007 0.037 0.036
0.006 0.019 0.001

atensor 8 H
2.985 -2.100 3.251
-2.100 1.361 -2.228
3.251 -2.228 3.608
0.006 0.017 -0.038
0.017 0.019 0.026
-0.007 0.005 -0.001

atensor 9 C
-1.295 -0.404 1.498
-0.404 -1.607 -1.027
1.498 -1.027 0.444
0.043 0.011 -0.031
0.011 0.052 0.021
-0.016 0.011 0.001

atensor 10 H
2.750 2.176 3.124
2.176 1.595 2.403
3.124 2.403 3.608
0.008 -0.018 -0.037
-0.018 0.017 -0.028
-0.007 -0.005 -0.001

atensor 11 C
-1.341 0.418 1.440
0.418 -1.563 1.108

1.440 1.108 0.443
0.044 -0.012 -0.029
-0.012 0.051 -0.023
-0.016 -0.012 0.001

atensor 12 H
0.281 1.222 1.115
1.222 4.064 3.780
1.115 3.780 3.608
0.028 -0.010 -0.013
-0.010 -0.003 -0.044
-0.002 -0.008 -0.001

atensor 13 C
-1.816 0.235 0.514
0.235 -1.089 1.742
0.514 1.742 0.443
0.058 -0.007 -0.011
-0.007 0.037 -0.036
-0.006 -0.019 0.001

atensor 14 H
2.985 -2.100 -3.251
-2.100 1.360 2.228
-3.251 2.228 3.608
0.006 0.017 0.038
0.017 0.019 -0.026
0.007 -0.005 -0.001

atensor 15 C
-1.296 -0.403 -1.498
-0.403 -1.608 1.027
-1.498 1.027 0.443
0.043 0.011 0.031
0.011 0.052 -0.021
0.016 -0.011 0.001

atensor 16 H
2.750 2.177 -3.124
2.177 1.596 -2.403
-3.123 -2.403 3.607
0.008 -0.018 0.037
-0.018 0.017 0.028
0.007 0.005 -0.001

atensor 17 C
-1.341 0.418 -1.440
0.418 -1.563 -1.108
-1.440 -1.108 0.443
0.044 -0.012 0.029
-0.012 0.051 0.023
0.016 0.012 0.001

atensor 18 H
0.427 -1.422 1.320
-1.422 3.920 -3.713
1.320 -3.713 3.607
0.027 0.012 -0.016
0.012 -0.002 0.044
-0.003 0.008 -0.001

atensor 19 C
-1.787 -0.273 0.608
-0.273 -1.116 -1.712
0.608 -1.712 0.443
0.057 0.008 -0.012
0.008 0.038 0.035

-0.007 0.019 0.001

atensor 20 C

-1.020 0.024 1.816
0.024 -1.884 0.050
1.816 0.050 0.442
0.036 -0.001 -0.037
-0.001 0.059 -0.001
-0.020 -0.001 0.001

atensor 21 H

4.421 0.123 3.940
0.123 -0.076 0.108
3.940 0.108 3.607
-0.006 -0.001 -0.046
-0.001 0.031 -0.001
-0.009 0.000 -0.001

orbtensor 1 V

-4705.509 0.013 -0.029
0.013 -4705.508 -0.243
-0.029 -0.243 -170.290
1698.714 0.000 0.000
0.000 1698.714 -0.001
0.000 -0.001 1714.685

orbtensor 2 H

-0.740 4.679 1.038
4.679 -12.236 -2.919
1.038 -2.919 -0.534
28.086 -4.789 -0.935
-4.789 39.853 2.631
-0.935 2.631 25.509

orbtensor 3 C

-182.398 18.853 8.630
18.853 -228.718 -24.288
8.630 -24.288 -64.818
255.483 2.934 -1.454
2.934 248.274 4.091
-1.454 4.091 232.307

orbtensor 4 H

-13.889 -0.407 3.096
-0.407 0.913 0.085
3.096 0.085 -0.533
41.545 0.416 -2.790
0.416 26.395 -0.076
-2.790 -0.076 25.508

orbtensor 5 C

-235.378 -1.637 25.758
-1.637 -175.740 0.704
25.758 0.704 -64.815
247.239 -0.255 -4.339
-0.255 256.519 -0.118
-4.339 -0.118 232.307

orbtensor 6 H

-0.261 -4.022 0.876
-4.022 -12.714 2.971
0.876 2.971 -0.533
27.596 4.116 -0.790
4.116 40.343 -2.678
-0.790 -2.678 25.508

orbtensor 7 C

```
-180.472  -16.205   7.284
-16.205  -230.644  24.717
7.284    24.717  -64.816
255.782  -2.521   -1.227
-2.521   247.976  -4.164
-1.227   -4.164  232.307
```

```
orbtensor 8 H
-9.161    6.914   -2.556
6.914   -3.813    1.752
-2.556    1.752   -0.533
36.706   -7.077    2.304
-7.077   31.232   -1.579
2.304   -1.579   25.508
```

```
orbtensor 9 C
-216.326  27.854  -21.265
27.854 -194.784  14.569
-21.265  14.569  -64.819
250.203  4.333   3.582
4.333  253.555  -2.454
3.582  -2.454  232.308
```

```
orbtensor 10 H
-8.388   -7.164   -2.456
-7.164   -4.587   -1.890
-2.456   -1.890   -0.533
35.914    7.333    2.214
7.333   32.023    1.703
2.214    1.703   25.508
```

```
orbtensor 11 C
-213.210  -28.865  -20.436
-28.865 -197.899  -15.720
-20.436 -15.720  -64.821
250.686  -4.492    3.441
-4.492  253.070    2.648
3.441    2.648  232.308
```

```
orbtensor 12 H
-0.261   -4.022   -0.877
-4.022  -12.714   -2.973
-0.877   -2.973   -0.533
27.596    4.116    0.790
4.116   40.342    2.679
0.790    2.679   25.508
```

```
orbtensor 13 C
-180.471  -16.204  -7.287
-16.204 -230.639  -24.733
-7.287  -24.733  -64.821
255.782  -2.521    1.228
-2.521  247.975    4.165
1.228    4.165  232.308
```

```
orbtensor 14 H
-9.161    6.913    2.557
6.913   -3.813   -1.752
2.557   -1.752   -0.533
36.706   -7.076   -2.304
-7.076   31.232    1.580
-2.304    1.580   25.508
```

```
orbtensor 15 C
-216.327  27.852  21.263
27.852 -194.780  -14.582
21.263 -14.582  -64.821
```

250.202	4.334	-3.581
4.334	253.554	2.456
-3.581	2.456	232.308

orbtensor 16 H

-8.388	-7.165	2.455
-7.165	-4.587	1.889
2.455	1.889	-0.533
35.915	7.333	-2.213
7.333	32.024	-1.702
-2.213	-1.702	25.508

orbtensor 17 C

-213.212	-28.868	20.428
-28.868	-197.903	15.705
20.428	15.705	-64.816
250.687	-4.491	-3.441
-4.491	253.071	-2.646
-3.441	-2.646	232.307

orbtensor 18 H

-0.740	4.679	-1.037
4.679	-12.237	2.918
-1.037	2.918	-0.533
28.086	-4.789	0.935
-4.789	39.854	-2.629
0.935	-2.629	25.508

orbtensor 19 C

-182.397	18.854	-8.629
18.854	-228.722	24.269
-8.629	24.269	-64.813
255.484	2.934	1.454
2.934	248.275	-4.089
1.454	-4.089	232.306

orbtensor 20 C

-235.379	-1.635	-25.758
-1.635	-175.739	-0.716
-25.758	-0.716	-64.816
247.238	-0.255	4.339
-0.255	256.519	0.121
4.339	0.121	232.306

orbtensor 21 H

-13.889	-0.406	-3.096
-0.406	0.913	-0.085
-3.096	-0.085	-0.533
41.545	0.416	2.790
0.416	26.395	0.077
2.790	0.077	25.508

gtensor (ppt)

-0.148	0.000	0.000
0.000	-0.148	0.000
0.000	0.000	-0.132
-18.039	0.000	0.000
0.000	-18.039	-0.001
0.000	-0.001	-0.624

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
---	----	------------	---------------	-----------	-----------	--------------	---------

1	V	-78.7317	-1489.73133	39367.26678	51.15812	39418.42489	37928.69356
2	H	2.6590	26.64600	-350.15199	-0.36396	-350.51595	-323.86995
3	C	-0.7890	86.71000	413.11617	-1.88321	411.23296	497.94296
4	H	2.6587	26.64633	-350.10809	-0.36426	-350.47235	-323.82602
5	C	-0.7877	86.71067	412.41804	-1.88300	410.53504	497.24570
6	H	2.6587	26.64633	-350.10809	-0.36442	-350.47251	-323.82618
7	C	-0.7870	86.71100	412.06898	-1.88380	410.18517	496.89617
8	H	2.6593	26.64633	-350.19588	-0.36448	-350.56036	-323.91403
9	C	-0.7873	86.71233	412.24351	-1.88419	410.35932	497.07165
10	H	2.6590	26.64567	-350.15199	-0.36440	-350.51639	-323.87073
11	C	-0.7883	86.71133	412.76710	-1.88382	410.88328	497.59461
12	H	2.6590	26.64600	-350.15199	-0.36434	-350.51633	-323.87033
13	C	-0.7887	86.71133	412.94163	-1.88422	411.05741	497.76875
14	H	2.6590	26.64633	-350.15199	-0.36441	-350.51640	-323.87007
15	C	-0.7883	86.71200	412.76710	-1.88384	410.88327	497.59527
16	H	2.6590	26.64633	-350.15199	-0.36423	-350.51622	-323.86988
17	C	-0.7883	86.71133	412.76710	-1.88420	410.88290	497.59423
18	H	2.6593	26.64600	-350.19588	-0.36416	-350.56004	-323.91404
19	C	-0.7880	86.71100	412.59257	-1.88380	410.70877	497.41977
20	C	-0.7887	86.70967	412.94163	-1.88299	411.05865	497.76832
21	H	2.6587	26.64633	-350.10809	-0.36425	-350.47234	-323.82601
13C Average		-0.7881	86.71107	412.66238	-1.88371	410.77868	497.48974
1H Average		2.6590	26.64617	-350.14760	-0.36429	-350.51189	-323.86572

=====
4VCp2-STO-BHLYP-ORCA
Temperature: 298
Spin: 1.5

atensor 1 V
-48.726 0.000 0.000
0.000 -48.727 0.004
0.000 0.004 -110.036
-12.485 0.000 0.000
0.000 -12.485 0.000
0.000 0.000 -3.736

atensor 2 H
0.427 -1.422 -1.320
-1.422 3.919 3.713
-1.320 3.713 3.607
0.027 0.012 0.016
0.012 -0.002 -0.044
0.003 -0.008 -0.001

atensor 3 C
-1.788 -0.273 -0.608
-0.273 -1.117 1.711
-0.608 1.711 0.442
0.057 0.008 0.012
0.008 0.038 -0.035
0.007 -0.019 0.001

atensor 4 H
4.421 0.124 -3.940
0.124 -0.076 -0.108
-3.940 -0.108 3.607
-0.006 -0.001 0.046
-0.001 0.031 0.001
0.009 0.000 -0.001

atensor 5 C
-1.019 0.024 -1.816
0.024 -1.883 -0.050
-1.816 -0.050 0.443

0.036 -0.001 0.037
-0.001 0.059 0.001
0.020 0.001 0.001

atensor 6 H
0.281 1.222 -1.115
1.222 4.064 -3.780
-1.115 -3.780 3.607
0.028 -0.010 0.013
-0.010 -0.003 0.044
0.002 0.008 -0.001

atensor 7 C
-1.814 0.235 -0.514
0.235 -1.087 -1.742
-0.514 -1.742 0.444
0.058 -0.007 0.011
-0.007 0.037 0.036
0.006 0.019 0.001

atensor 8 H
2.985 -2.100 3.251
-2.100 1.361 -2.228
3.251 -2.228 3.608
0.006 0.017 -0.038
0.017 0.019 0.026
-0.007 0.005 -0.001

atensor 9 C
-1.295 -0.404 1.498
-0.404 -1.607 -1.027
1.498 -1.027 0.444
0.043 0.011 -0.031
0.011 0.052 0.021
-0.016 0.011 0.001

atensor 10 H
2.750 2.176 3.124
2.176 1.595 2.403
3.124 2.403 3.608
0.008 -0.018 -0.037
-0.018 0.017 -0.028
-0.007 -0.005 -0.001

atensor 11 C
-1.341 0.418 1.440
0.418 -1.563 1.108
1.440 1.108 0.443
0.044 -0.012 -0.029
-0.012 0.051 -0.023
-0.016 -0.012 0.001

atensor 12 H
0.281 1.222 1.115
1.222 4.064 3.780
1.115 3.780 3.608
0.028 -0.010 -0.013
-0.010 -0.003 -0.044
-0.002 -0.008 -0.001

atensor 13 C
-1.816 0.235 0.514
0.235 -1.089 1.742
0.514 1.742 0.443
0.058 -0.007 -0.011
-0.007 0.037 -0.036
-0.006 -0.019 0.001

atensor 14 H
2.985 -2.100 -3.251
-2.100 1.360 2.228
-3.251 2.228 3.608
0.006 0.017 0.038
0.017 0.019 -0.026
0.007 -0.005 -0.001

atensor 15 C
-1.296 -0.403 -1.498
-0.403 -1.608 1.027
-1.498 1.027 0.443
0.043 0.011 0.031
0.011 0.052 -0.021
0.016 -0.011 0.001

atensor 16 H
2.750 2.177 -3.124
2.177 1.596 -2.403
-3.123 -2.403 3.607
0.008 -0.018 0.037
-0.018 0.017 0.028
0.007 0.005 -0.001

atensor 17 C
-1.341 0.418 -1.440
0.418 -1.563 -1.108
-1.440 -1.108 0.443
0.044 -0.012 0.029
-0.012 0.051 0.023
0.016 0.012 0.001

atensor 18 H
0.427 -1.422 1.320
-1.422 3.920 -3.713
1.320 -3.713 3.607
0.027 0.012 -0.016
0.012 -0.002 0.044
-0.003 0.008 -0.001

atensor 19 C
-1.787 -0.273 0.608
-0.273 -1.116 -1.712
0.608 -1.712 0.443
0.057 0.008 -0.012
0.008 0.038 0.035
-0.007 0.019 0.001

atensor 20 C
-1.020 0.024 1.816
0.024 -1.884 0.050
1.816 0.050 0.442
0.036 -0.001 -0.037
-0.001 0.059 -0.001
-0.020 -0.001 0.001

atensor 21 H
4.421 0.123 3.940
0.123 -0.076 0.108
3.940 0.108 3.607
-0.006 -0.001 -0.046
-0.001 0.031 -0.001
-0.009 0.000 -0.001

orbtensor 1 V
-4705.509 0.013 -0.029

0.013 -4705.508 -0.243
-0.029 -0.243 -170.290
1698.714 0.000 0.000
0.000 1698.714 -0.001
0.000 -0.001 1714.685

orbtensor 2 H
-0.740 4.679 1.038
4.679 -12.236 -2.919
1.038 -2.919 -0.534
28.086 -4.789 -0.935
-4.789 39.853 2.631
-0.935 2.631 25.509

orbtensor 3 C
-182.398 18.853 8.630
18.853 -228.718 -24.288
8.630 -24.288 -64.818
255.483 2.934 -1.454
2.934 248.274 4.091
-1.454 4.091 232.307

orbtensor 4 H
-13.889 -0.407 3.096
-0.407 0.913 0.085
3.096 0.085 -0.533
41.545 0.416 -2.790
0.416 26.395 -0.076
-2.790 -0.076 25.508

orbtensor 5 C
-235.378 -1.637 25.758
-1.637 -175.740 0.704
25.758 0.704 -64.815
247.239 -0.255 -4.339
-0.255 256.519 -0.118
-4.339 -0.118 232.307

orbtensor 6 H
-0.261 -4.022 0.876
-4.022 -12.714 2.971
0.876 2.971 -0.533
27.596 4.116 -0.790
4.116 40.343 -2.678
-0.790 -2.678 25.508

orbtensor 7 C
-180.472 -16.205 7.284
-16.205 -230.644 24.717
7.284 24.717 -64.816
255.782 -2.521 -1.227
-2.521 247.976 -4.164
-1.227 -4.164 232.307

orbtensor 8 H
-9.161 6.914 -2.556
6.914 -3.813 1.752
-2.556 1.752 -0.533
36.706 -7.077 2.304
-7.077 31.232 -1.579
2.304 -1.579 25.508

orbtensor 9 C
-216.326 27.854 -21.265
27.854 -194.784 14.569
-21.265 14.569 -64.819
250.203 4.333 3.582

4.333 253.555 -2.454
3.582 -2.454 232.308

orbtensor 10 H
-8.388 -7.164 -2.456
-7.164 -4.587 -1.890
-2.456 -1.890 -0.533
35.914 7.333 2.214
7.333 32.023 1.703
2.214 1.703 25.508

orbtensor 11 C
-213.210 -28.865 -20.436
-28.865 -197.899 -15.720
-20.436 -15.720 -64.821
250.686 -4.492 3.441
-4.492 253.070 2.648
3.441 2.648 232.308

orbtensor 12 H
-0.261 -4.022 -0.877
-4.022 -12.714 -2.973
-0.877 -2.973 -0.533
27.596 4.116 0.790
4.116 40.342 2.679
0.790 2.679 25.508

orbtensor 13 C
-180.471 -16.204 -7.287
-16.204 -230.639 -24.733
-7.287 -24.733 -64.821
255.782 -2.521 1.228
-2.521 247.975 4.165
1.228 4.165 232.308

orbtensor 14 H
-9.161 6.913 2.557
6.913 -3.813 -1.752
2.557 -1.752 -0.533
36.706 -7.076 -2.304
-7.076 31.232 1.580
-2.304 1.580 25.508

orbtensor 15 C
-216.327 27.852 21.263
27.852 -194.780 -14.582
21.263 -14.582 -64.821
250.202 4.334 -3.581
4.334 253.554 2.456
-3.581 2.456 232.308

orbtensor 16 H
-8.388 -7.165 2.455
-7.165 -4.587 1.889
2.455 1.889 -0.533
35.915 7.333 -2.213
7.333 32.024 -1.702
-2.213 -1.702 25.508

orbtensor 17 C
-213.212 -28.868 20.428
-28.868 -197.903 15.705
20.428 15.705 -64.816
250.687 -4.491 -3.441
-4.491 253.071 -2.646
-3.441 -2.646 232.307

```

orbtensor 18 H
-0.740  4.679  -1.037
4.679 -12.237  2.918
-1.037  2.918  -0.533
28.086  -4.789  0.935
-4.789  39.854  -2.629
0.935  -2.629  25.508

```

```

orbtensor 19 C
-182.397  18.854  -8.629
18.854 -228.722  24.269
-8.629  24.269  -64.813
255.484  2.934  1.454
2.934  248.275  -4.089
1.454  -4.089  232.306

```

```

orbtensor 20 C
-235.379  -1.635  -25.758
-1.635 -175.739  -0.716
-25.758  -0.716  -64.816
247.238  -0.255  4.339
-0.255  256.519  0.121
4.339  0.121  232.306

```

```

orbtensor 21 H
-13.889  -0.406  -3.096
-0.406  0.913  -0.085
-3.096  -0.085  -0.533
41.545  0.416  2.790
0.416  26.395  0.077
2.790  0.077  25.508

```

```

gtensor (ppt)
-0.148  0.000  0.000
0.000  -0.148  0.000
0.000  0.000  -0.132
-18.039  0.000  0.000
0.000  -18.039  -0.001
0.000  -0.001  -0.624

```

```

zfstensor (cm-1)
-0.684893  0.000016  -0.000017
0.000016  -0.685169  -0.000104
-0.000017  -0.000104  1.356776

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-78.7317	-1489.73133	39365.85169	-18.01672	39347.83497	37858.10364
2	H	2.6590	26.64600	-350.13940	0.12808	-350.01132	-323.36532
3	C	-0.7890	86.71000	413.10132	0.66319	413.76450	500.47450
4	H	2.6587	26.64633	-350.09551	0.12847	-349.96704	-323.32070
5	C	-0.7877	86.71067	412.40321	0.66333	413.06654	499.77721
6	H	2.6587	26.64633	-350.09551	0.12820	-349.96731	-323.32097
7	C	-0.7870	86.71100	412.05416	0.66331	412.71748	499.42848
8	H	2.6593	26.64633	-350.18330	0.12836	-350.05494	-323.40861
9	C	-0.7873	86.71233	412.22869	0.66352	412.89221	499.60454
10	H	2.6590	26.64567	-350.13940	0.12838	-350.01102	-323.36535
11	C	-0.7883	86.71133	412.75226	0.66346	413.41573	500.12706
12	H	2.6590	26.64600	-350.13940	0.12821	-350.01120	-323.36520
13	C	-0.7887	86.71133	412.92679	0.66352	413.59031	500.30164
14	H	2.6590	26.64633	-350.13940	0.12842	-350.01098	-323.36465

15	C	-0.7883	86.71200	412.75226	0.66355	413.41582	500.12782
16	H	2.6590	26.64633	-350.13940	0.12834	-350.01106	-323.36473
17	C	-0.7883	86.71133	412.75226	0.66364	413.41590	500.12723
18	H	2.6593	26.64600	-350.18330	0.12808	-350.05522	-323.40922
19	C	-0.7880	86.71100	412.57774	0.66327	413.24101	499.95201
20	C	-0.7887	86.70967	412.92679	0.66320	413.58999	500.29966
21	H	2.6587	26.64633	-350.09551	0.12840	-349.96711	-323.32077
13C Average		-0.7881	86.71107	412.64755	0.66340	413.31095	500.02201
1H Average		2.6590	26.64617	-350.13501	0.12829	-350.00672	-323.36055

=====
 4VCp2-STO-BP-No-ZFS

Temperature: 298

Spin: 1.5

atensor 1 V

30.492 0.000 0.000
 0.000 30.492 0.004
 0.000 0.004 -26.547
 -8.141 0.000 0.000
 0.000 -8.141 0.000
 0.000 0.000 -4.908

atensor 2 H

0.789 -1.392 -1.265
 -1.392 4.207 3.558
 -1.265 3.558 4.124
 0.013 0.003 0.007
 0.003 0.006 -0.020
 0.004 -0.011 -0.003

atensor 3 C

-1.711 -0.244 -0.593
 -0.244 -1.112 1.667
 -0.593 1.667 0.606
 0.046 0.006 0.007
 0.006 0.030 -0.019
 0.007 -0.020 0.000

atensor 4 H

4.699 0.121 -3.775
 0.121 0.297 -0.104
 -3.775 -0.104 4.123
 0.004 0.000 0.021
 0.000 0.015 0.001
 0.012 0.000 -0.003

atensor 5 C

-1.024 0.021 -1.769
 0.021 -1.797 -0.049
 -1.769 -0.049 0.607
 0.028 -0.001 0.020
 -0.001 0.048 0.001
 0.021 0.001 0.000

atensor 6 H

0.646 1.196 -1.068
 1.196 4.350 -3.622
 -1.068 -3.622 4.124
 0.014 -0.003 0.006
 -0.003 0.005 0.020
 0.003 0.011 -0.003

atensor 7 C

-1.735 0.210 -0.501
 0.210 -1.085 -1.698

-0.501 -1.698 0.608
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.293 -2.056 3.115
-2.056 1.703 -2.135
3.115 -2.135 4.124
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.271 -0.361 1.460
-0.361 -1.550 -1.001
1.460 -1.001 0.608
0.034 0.010 -0.016
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.063 2.130 2.993
2.130 1.933 2.303
2.993 2.303 4.124
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.312 0.374 1.403
0.374 -1.511 1.079
1.403 1.079 0.607
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.016 -0.013 0.000

atensor 12 H
0.646 1.196 1.068
1.196 4.349 3.622
1.068 3.622 4.125
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.736 0.210 0.501
0.210 -1.086 1.698
0.501 1.698 0.607
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.293 -2.056 -3.115
-2.056 1.703 2.135
-3.115 2.135 4.125
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.271 -0.361 -1.460
-0.361 -1.550 1.001
-1.460 1.000 0.608
0.034 0.010 0.016
0.010 0.042 -0.011

0.017 -0.012 0.000

atensor 16 H
3.063 2.131 -2.993
2.131 1.933 -2.303
-2.993 -2.303 4.124
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.312 0.374 -1.403
0.374 -1.510 -1.079
-1.403 -1.079 0.607
0.035 -0.010 0.016
-0.010 0.041 0.012
0.016 0.013 0.000

atensor 18 H
0.788 -1.392 1.265
-1.392 4.208 -3.558
1.265 -3.558 4.123
0.013 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.711 -0.244 0.593
-0.244 -1.111 -1.668
0.593 -1.668 0.607
0.046 0.006 -0.007
0.006 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.025 0.021 1.769
0.021 -1.797 0.048
1.769 0.048 0.606
0.028 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.698 0.121 3.775
0.121 0.296 0.103
3.775 0.103 4.123
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3063.695 -0.014 -0.020
-0.014 -3063.683 -0.148
-0.020 -0.148 -351.484
1708.729 0.000 0.000
0.000 1708.729 -0.001
0.000 -0.001 1716.839

orbtensor 2 H
-1.248 3.381 0.961
3.381 -9.554 -2.702
0.961 -2.702 -0.687
26.492 -4.356 -1.274
-4.356 37.194 3.582
-1.274 3.582 25.670

orbtensor 3 C

-158.398	23.568	10.503
23.568	-216.303	-29.554
10.503	-29.554	-60.849
228.012	-5.093	-4.490
-5.093	240.524	12.628
-4.490	12.628	223.286

orbtensor 4 H

-10.748	-0.294	2.866
-0.294	-0.054	0.079
2.866	0.079	-0.686
38.733	0.379	-3.800
0.379	24.954	-0.104
-3.800	-0.104	25.669

orbtensor 5 C

-224.630	-2.048	31.345
-2.048	-150.070	0.857
31.345	0.857	-60.845
242.324	0.443	-13.396
0.443	226.213	-0.368
-13.396	-0.368	223.283

orbtensor 6 H

-0.904	-2.905	0.811
-2.905	-9.899	2.751
0.811	2.751	-0.686
26.048	3.744	-1.075
3.744	37.640	-3.646
-1.075	-3.646	25.669

orbtensor 7 C

-155.990	-20.258	8.866
-20.258	-218.715	30.079
8.866	30.079	-60.846
227.493	4.378	-3.790
4.378	241.048	-12.854
-3.790	-12.854	223.283

orbtensor 8 H

-7.333	4.994	-2.366
4.994	-3.470	1.622
-2.366	1.622	-0.687
34.332	-6.435	3.136
-6.435	29.355	-2.150
3.136	-2.150	25.669

orbtensor 9 C

-200.816	34.822	-25.874
34.822	-173.885	17.732
-25.874	17.732	-60.848
237.180	-7.524	11.055
-7.524	231.361	-7.577
11.055	-7.577	223.284

orbtensor 10 H

-6.774	-5.176	-2.274
-5.176	-4.028	-1.749
-2.274	-1.749	-0.687
33.612	6.669	3.014
6.669	30.074	2.318
3.014	2.318	25.670

orbtensor 11 C

-196.923	-36.084	-24.865
-36.084	-177.780	-19.129
-24.865	-19.129	-60.850

236.337	7.797	10.623
7.797	232.200	8.172
10.623	8.172	223.285

orbtensor 12 H

-0.903	-2.905	-0.811
-2.905	-9.899	-2.751
-0.811	-2.751	-0.687
26.047	3.743	1.075
3.743	37.639	3.647
1.075	3.647	25.670

orbtensor 13 C

-155.986	-20.258	-8.868
-20.258	-218.707	-30.094
-8.868	-30.094	-60.852
227.493	4.377	3.790
4.377	241.043	12.856
3.790	12.856	223.287

orbtensor 14 H

-7.332	4.994	2.366
4.994	-3.469	-1.622
2.366	-1.622	-0.687
34.332	-6.435	-3.136
-6.435	29.354	2.150
-3.136	2.150	25.670

orbtensor 15 C

-200.816	34.818	25.874
34.818	-173.880	-17.742
25.874	-17.742	-60.852
237.179	-7.522	-11.055
-7.522	231.358	7.577
-11.055	7.577	223.287

orbtensor 16 H

-6.774	-5.176	2.273
-5.176	-4.029	1.749
2.273	1.749	-0.687
33.613	6.669	-3.013
6.669	30.075	-2.318
-3.013	-2.318	25.669

orbtensor 17 C

-196.924	-36.087	24.857
-36.087	-177.785	19.114
24.857	19.114	-60.844
236.337	7.798	-10.622
7.798	232.202	-8.171
-10.622	-8.171	223.283

orbtensor 18 H

-1.248	3.381	-0.960
3.381	-9.554	2.701
-0.960	2.701	-0.686
26.492	-4.356	1.273
-4.356	37.195	-3.581
1.273	-3.581	25.669

orbtensor 19 C

-158.399	23.568	-10.502
23.568	-216.310	29.537
-10.502	29.537	-60.842
228.013	-5.093	4.489
-5.093	240.527	-12.626
4.489	-12.626	223.282


```

orbtensor 20 C
-224.629  -2.045  -31.346
-2.045  -150.069  -0.867
-31.346  -0.867  -60.846
242.323  0.441  13.396
0.441  226.212  0.368
13.396  0.368  223.283

```

```

orbtensor 21 H
-10.748  -0.293  -2.867
-0.293  -0.054  -0.079
-2.867  -0.079  -0.687
38.733  0.378  3.800
0.378  24.954  0.104
3.800  0.104  25.669

```

```

gtensor (ppt)
-0.125  0.000  0.000
0.000  -0.125  0.000
0.000  0.000  -0.131
-6.329  0.000  0.000
0.000  -6.329  0.000
0.000  0.000  -1.270

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	4.4157	-448.18833	-2216.35397	15.18143	-2201.17254	-2649.36087
2	H	3.0453	25.95567	-402.55954	-0.11990	-402.67943	-376.72377
3	C	-0.7137	85.42400	375.10048	-0.58485	374.51563	459.93963
4	H	3.0450	25.95600	-402.51547	-0.11982	-402.63529	-376.67929
5	C	-0.7127	85.42500	374.57488	-0.58485	373.99003	459.41503
6	H	3.0453	25.95600	-402.55954	-0.11990	-402.67943	-376.72343
7	C	-0.7120	85.42433	374.22449	-0.58500	373.63949	459.06382
8	H	3.0453	25.95533	-402.55954	-0.11990	-402.67943	-376.72410
9	C	-0.7123	85.42533	374.39969	-0.58515	373.81454	459.23987
10	H	3.0453	25.95567	-402.55954	-0.11990	-402.67943	-376.72377
11	C	-0.7133	85.42300	374.92528	-0.58515	374.34013	459.76313
12	H	3.0453	25.95567	-402.55954	-0.12001	-402.67954	-376.72388
13	C	-0.7130	85.42600	374.75008	-0.58500	374.16508	459.59108
14	H	3.0457	25.95600	-402.60360	-0.11997	-402.72357	-376.76757
15	C	-0.7123	85.42533	374.39969	-0.58515	373.81454	459.23987
16	H	3.0453	25.95567	-402.55954	-0.11990	-402.67943	-376.72377
17	C	-0.7130	85.42300	374.75008	-0.58500	374.16508	459.58808
18	H	3.0450	25.95600	-402.51547	-0.11982	-402.63529	-376.67929
19	C	-0.7130	85.42367	374.75008	-0.58500	374.16508	459.58875
20	C	-0.7133	85.42467	374.92528	-0.58471	374.34058	459.76524
21	H	3.0443	25.95567	-402.42735	-0.11990	-402.54724	-376.59158
13C Average		-0.7129	85.42443	374.68000	-0.58499	374.09502	459.51945
1H Average		3.0452	25.95577	-402.54191	-0.11990	-402.66181	-376.70604

```

=====
4VCp2-STO-BP-Neese
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
30.492 0.000 0.000
0.000 30.492 0.004
0.000 0.004 -26.547

```

-8.141 0.000 0.000
0.000 -8.141 0.000
0.000 0.000 -4.908

atensor 2 H
0.789 -1.392 -1.265
-1.392 4.207 3.558
-1.265 3.558 4.124
0.013 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

atensor 3 C
-1.711 -0.244 -0.593
-0.244 -1.112 1.667
-0.593 1.667 0.606
0.046 0.006 0.007
0.006 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H
4.699 0.121 -3.775
0.121 0.297 -0.104
-3.775 -0.104 4.123
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C
-1.024 0.021 -1.769
0.021 -1.797 -0.049
-1.769 -0.049 0.607
0.028 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.646 1.196 -1.068
1.196 4.350 -3.622
-1.068 -3.622 4.124
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.735 0.210 -0.501
0.210 -1.085 -1.698
-0.501 -1.698 0.608
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.293 -2.056 3.115
-2.056 1.703 -2.135
3.115 -2.135 4.124
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.271 -0.361 1.460
-0.361 -1.550 -1.001
1.460 -1.001 0.608
0.034 0.010 -0.016
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.063 2.130 2.993
2.130 1.933 2.303
2.993 2.303 4.124
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.312 0.374 1.403
0.374 -1.511 1.079
1.403 1.079 0.607
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.016 -0.013 0.000

atensor 12 H
0.646 1.196 1.068
1.196 4.349 3.622
1.068 3.622 4.125
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.736 0.210 0.501
0.210 -1.086 1.698
0.501 1.698 0.607
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.293 -2.056 -3.115
-2.056 1.703 2.135
-3.115 2.135 4.125
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.271 -0.361 -1.460
-0.361 -1.550 1.001
-1.460 1.000 0.608
0.034 0.010 0.016
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.063 2.131 -2.993
2.131 1.933 -2.303
-2.993 -2.303 4.124
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.312 0.374 -1.403
0.374 -1.510 -1.079
-1.403 -1.079 0.607
0.035 -0.010 0.016
-0.010 0.041 0.012
0.016 0.013 0.000

atensor 18 H
0.788 -1.392 1.265

-1.392 4.208 -3.558
1.265 -3.558 4.123
0.013 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.711 -0.244 0.593
-0.244 -1.111 -1.668
0.593 -1.668 0.607
0.046 0.006 -0.007
0.006 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.025 0.021 1.769
0.021 -1.797 0.048
1.769 0.048 0.606
0.028 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.698 0.121 3.775
0.121 0.296 0.103
3.775 0.103 4.123
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3063.695 -0.014 -0.020
-0.014 -3063.683 -0.148
-0.020 -0.148 -351.484
1708.729 0.000 0.000
0.000 1708.729 -0.001
0.000 -0.001 1716.839

orbtensor 2 H
-1.248 3.381 0.961
3.381 -9.554 -2.702
0.961 -2.702 -0.687
26.492 -4.356 -1.274
-4.356 37.194 3.582
-1.274 3.582 25.670

orbtensor 3 C
-158.398 23.568 10.503
23.568 -216.303 -29.554
10.503 -29.554 -60.849
228.012 -5.093 -4.490
-5.093 240.524 12.628
-4.490 12.628 223.286

orbtensor 4 H
-10.748 -0.294 2.866
-0.294 -0.054 0.079
2.866 0.079 -0.686
38.733 0.379 -3.800
0.379 24.954 -0.104
-3.800 -0.104 25.669

orbtensor 5 C
-224.630 -2.048 31.345
-2.048 -150.070 0.857
31.345 0.857 -60.845
242.324 0.443 -13.396

0.443 226.213 -0.368
-13.396 -0.368 223.283

orbtensor 6 H
-0.904 -2.905 0.811
-2.905 -9.899 2.751
0.811 2.751 -0.686
26.048 3.744 -1.075
3.744 37.640 -3.646
-1.075 -3.646 25.669

orbtensor 7 C
-155.990 -20.258 8.866
-20.258 -218.715 30.079
8.866 30.079 -60.846
227.493 4.378 -3.790
4.378 241.048 -12.854
-3.790 -12.854 223.283

orbtensor 8 H
-7.333 4.994 -2.366
4.994 -3.470 1.622
-2.366 1.622 -0.687
34.332 -6.435 3.136
-6.435 29.355 -2.150
3.136 -2.150 25.669

orbtensor 9 C
-200.816 34.822 -25.874
34.822 -173.885 17.732
-25.874 17.732 -60.848
237.180 -7.524 11.055
-7.524 231.361 -7.577
11.055 -7.577 223.284

orbtensor 10 H
-6.774 -5.176 -2.274
-5.176 -4.028 -1.749
-2.274 -1.749 -0.687
33.612 6.669 3.014
6.669 30.074 2.318
3.014 2.318 25.670

orbtensor 11 C
-196.923 -36.084 -24.865
-36.084 -177.780 -19.129
-24.865 -19.129 -60.850
236.337 7.797 10.623
7.797 232.200 8.172
10.623 8.172 223.285

orbtensor 12 H
-0.903 -2.905 -0.811
-2.905 -9.899 -2.751
-0.811 -2.751 -0.687
26.047 3.743 1.075
3.743 37.639 3.647
1.075 3.647 25.670

orbtensor 13 C
-155.986 -20.258 -8.868
-20.258 -218.707 -30.094
-8.868 -30.094 -60.852
227.493 4.377 3.790
4.377 241.043 12.856
3.790 12.856 223.287

```

orbtensor 14 H
-7.332   4.994   2.366
4.994  -3.469  -1.622
2.366  -1.622  -0.687
34.332  -6.435  -3.136
-6.435  29.354   2.150
-3.136   2.150  25.670

```

```

orbtensor 15 C
-200.816  34.818  25.874
34.818 -173.880 -17.742
25.874 -17.742 -60.852
237.179  -7.522 -11.055
-7.522  231.358   7.577
-11.055   7.577  223.287

```

```

orbtensor 16 H
-6.774  -5.176   2.273
-5.176  -4.029   1.749
2.273   1.749  -0.687
33.613   6.669  -3.013
6.669  30.075  -2.318
-3.013  -2.318  25.669

```

```

orbtensor 17 C
-196.924  -36.087  24.857
-36.087 -177.785  19.114
24.857  19.114 -60.844
236.337   7.798 -10.622
7.798  232.202  -8.171
-10.622  -8.171  223.283

```

```

orbtensor 18 H
-1.248   3.381  -0.960
3.381  -9.554   2.701
-0.960   2.701  -0.686
26.492  -4.356   1.273
-4.356  37.195  -3.581
1.273  -3.581  25.669

```

```

orbtensor 19 C
-158.399  23.568 -10.502
23.568 -216.310  29.537
-10.502  29.537 -60.842
228.013  -5.093   4.489
-5.093  240.527 -12.626
4.489  -12.626  223.282

```

```

orbtensor 20 C
-224.629  -2.045  -31.346
-2.045 -150.069  -0.867
-31.346  -0.867  -60.846
242.323   0.441  13.396
0.441  226.212   0.368
13.396   0.368  223.283

```

```

orbtensor 21 H
-10.748  -0.293  -2.867
-0.293  -0.054  -0.079
-2.867  -0.079  -0.687
38.733   0.378   3.800
0.378  24.954   0.104
3.800   0.104  25.669

```

```

gtensor (ppt)
-0.125   0.000   0.000
0.000  -0.125   0.000

```

```

0.000    0.000    -0.131
-6.329    0.000    0.000
 0.000   -6.329    0.000
 0.000    0.000   -1.270

```

```

zfstensor (cm-1)
-0.369883   -0.000001   -0.000007
-0.000001   -0.369884    0.000061
-0.000007    0.000061    0.739768

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	4.4157	-448.18833	-2216.33749	-23.40021	-2239.73769	-2687.92603
2	H	3.0453	25.95567	-402.55654	0.18492	-402.37162	-376.41596
3	C	-0.7137	85.42400	375.09769	0.90169	375.99938	461.42338
4	H	3.0450	25.95600	-402.51248	0.18470	-402.32778	-376.37178
5	C	-0.7127	85.42500	374.57210	0.90149	375.47359	460.89859
6	H	3.0453	25.95600	-402.55654	0.18469	-402.37185	-376.41585
7	C	-0.7120	85.42433	374.22170	0.90150	375.12321	460.54754
8	H	3.0453	25.95533	-402.55654	0.18473	-402.37181	-376.41648
9	C	-0.7123	85.42533	374.39690	0.90179	375.29869	460.72402
10	H	3.0453	25.95567	-402.55654	0.18486	-402.37168	-376.41601
11	C	-0.7133	85.42300	374.92249	0.90204	375.82454	461.24754
12	H	3.0453	25.95567	-402.55654	0.18508	-402.37146	-376.41579
13	C	-0.7130	85.42600	374.74730	0.90190	375.64920	461.07520
14	H	3.0457	25.95600	-402.60061	0.18500	-402.41561	-376.45961
15	C	-0.7123	85.42533	374.39690	0.90207	375.29898	460.72431
16	H	3.0453	25.95567	-402.55654	0.18474	-402.37180	-376.41613
17	C	-0.7130	85.42300	374.74730	0.90159	375.64889	461.07189
18	H	3.0450	25.95600	-402.51248	0.18457	-402.32791	-376.37191
19	C	-0.7130	85.42367	374.74730	0.90149	375.64879	461.07245
20	C	-0.7133	85.42467	374.92249	0.90123	375.82372	461.24839
21	H	3.0443	25.95567	-402.42435	0.18479	-402.23956	-376.28389
13C Average		-0.7129	85.42443	374.67722	0.90168	375.57890	461.00333
1H Average		3.0452	25.95577	-402.53892	0.18481	-402.35411	-376.39834

```

=====
4VCp2-STO-BP-ORCA
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
30.492 0.000 0.000
0.000 30.492 0.004
0.000 0.004 -26.547
-8.141 0.000 0.000
0.000 -8.141 0.000
0.000 0.000 -4.908

```

```

atensor 2 H
0.789 -1.392 -1.265
-1.392 4.207 3.558
-1.265 3.558 4.124
0.013 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

```

```

atensor 3 C
-1.711 -0.244 -0.593
-0.244 -1.112 1.667

```

-0.593 1.667 0.606
0.046 0.006 0.007
0.006 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H
4.699 0.121 -3.775
0.121 0.297 -0.104
-3.775 -0.104 4.123
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C
-1.024 0.021 -1.769
0.021 -1.797 -0.049
-1.769 -0.049 0.607
0.028 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.646 1.196 -1.068
1.196 4.350 -3.622
-1.068 -3.622 4.124
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.735 0.210 -0.501
0.210 -1.085 -1.698
-0.501 -1.698 0.608
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.293 -2.056 3.115
-2.056 1.703 -2.135
3.115 -2.135 4.124
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.271 -0.361 1.460
-0.361 -1.550 -1.001
1.460 -1.001 0.608
0.034 0.010 -0.016
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.063 2.130 2.993
2.130 1.933 2.303
2.993 2.303 4.124
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.312 0.374 1.403
0.374 -1.511 1.079
1.403 1.079 0.607
0.035 -0.010 -0.016
-0.010 0.041 -0.012

-0.016 -0.013 0.000

atensor 12 H
0.646 1.196 1.068
1.196 4.349 3.622
1.068 3.622 4.125
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.736 0.210 0.501
0.210 -1.086 1.698
0.501 1.698 0.607
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.293 -2.056 -3.115
-2.056 1.703 2.135
-3.115 2.135 4.125
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.271 -0.361 -1.460
-0.361 -1.550 1.001
-1.460 1.000 0.608
0.034 0.010 0.016
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.063 2.131 -2.993
2.131 1.933 -2.303
-2.993 -2.303 4.124
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.312 0.374 -1.403
0.374 -1.510 -1.079
-1.403 -1.079 0.607
0.035 -0.010 0.016
-0.010 0.041 0.012
0.016 0.013 0.000

atensor 18 H
0.788 -1.392 1.265
-1.392 4.208 -3.558
1.265 -3.558 4.123
0.013 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.711 -0.244 0.593
-0.244 -1.111 -1.668
0.593 -1.668 0.607
0.046 0.006 -0.007
0.006 0.030 0.019
-0.007 0.020 0.000

atensor 20 C

-1.025 0.021 1.769
0.021 -1.797 0.048
1.769 0.048 0.606
0.028 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.698 0.121 3.775
0.121 0.296 0.103
3.775 0.103 4.123
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3063.695 -0.014 -0.020
-0.014 -3063.683 -0.148
-0.020 -0.148 -351.484
1708.729 0.000 0.000
0.000 1708.729 -0.001
0.000 -0.001 1716.839

orbtensor 2 H
-1.248 3.381 0.961
3.381 -9.554 -2.702
0.961 -2.702 -0.687
26.492 -4.356 -1.274
-4.356 37.194 3.582
-1.274 3.582 25.670

orbtensor 3 C
-158.398 23.568 10.503
23.568 -216.303 -29.554
10.503 -29.554 -60.849
228.012 -5.093 -4.490
-5.093 240.524 12.628
-4.490 12.628 223.286

orbtensor 4 H
-10.748 -0.294 2.866
-0.294 -0.054 0.079
2.866 0.079 -0.686
38.733 0.379 -3.800
0.379 24.954 -0.104
-3.800 -0.104 25.669

orbtensor 5 C
-224.630 -2.048 31.345
-2.048 -150.070 0.857
31.345 0.857 -60.845
242.324 0.443 -13.396
0.443 226.213 -0.368
-13.396 -0.368 223.283

orbtensor 6 H
-0.904 -2.905 0.811
-2.905 -9.899 2.751
0.811 2.751 -0.686
26.048 3.744 -1.075
3.744 37.640 -3.646
-1.075 -3.646 25.669

orbtensor 7 C
-155.990 -20.258 8.866
-20.258 -218.715 30.079
8.866 30.079 -60.846

227.493	4.378	-3.790
4.378	241.048	-12.854
-3.790	-12.854	223.283

orbtensor 8 H

-7.333	4.994	-2.366
4.994	-3.470	1.622
-2.366	1.622	-0.687
34.332	-6.435	3.136
-6.435	29.355	-2.150
3.136	-2.150	25.669

orbtensor 9 C

-200.816	34.822	-25.874
34.822	-173.885	17.732
-25.874	17.732	-60.848
237.180	-7.524	11.055
-7.524	231.361	-7.577
11.055	-7.577	223.284

orbtensor 10 H

-6.774	-5.176	-2.274
-5.176	-4.028	-1.749
-2.274	-1.749	-0.687
33.612	6.669	3.014
6.669	30.074	2.318
3.014	2.318	25.670

orbtensor 11 C

-196.923	-36.084	-24.865
-36.084	-177.780	-19.129
-24.865	-19.129	-60.850
236.337	7.797	10.623
7.797	232.200	8.172
10.623	8.172	223.285

orbtensor 12 H

-0.903	-2.905	-0.811
-2.905	-9.899	-2.751
-0.811	-2.751	-0.687
26.047	3.743	1.075
3.743	37.639	3.647
1.075	3.647	25.670

orbtensor 13 C

-155.986	-20.258	-8.868
-20.258	-218.707	-30.094
-8.868	-30.094	-60.852
227.493	4.377	3.790
4.377	241.043	12.856
3.790	12.856	223.287

orbtensor 14 H

-7.332	4.994	2.366
4.994	-3.469	-1.622
2.366	-1.622	-0.687
34.332	-6.435	-3.136
-6.435	29.354	2.150
-3.136	2.150	25.670

orbtensor 15 C

-200.816	34.818	25.874
34.818	-173.880	-17.742
25.874	-17.742	-60.852
237.179	-7.522	-11.055
-7.522	231.358	7.577
-11.055	7.577	223.287

orbtensor 16 H
-6.774 -5.176 2.273
-5.176 -4.029 1.749
2.273 1.749 -0.687
33.613 6.669 -3.013
6.669 30.075 -2.318
-3.013 -2.318 25.669

orbtensor 17 C
-196.924 -36.087 24.857
-36.087 -177.785 19.114
24.857 19.114 -60.844
236.337 7.798 -10.622
7.798 232.202 -8.171
-10.622 -8.171 223.283

orbtensor 18 H
-1.248 3.381 -0.960
3.381 -9.554 2.701
-0.960 2.701 -0.686
26.492 -4.356 1.273
-4.356 37.195 -3.581
1.273 -3.581 25.669

orbtensor 19 C
-158.399 23.568 -10.502
23.568 -216.310 29.537
-10.502 29.537 -60.842
228.013 -5.093 4.489
-5.093 240.527 -12.626
4.489 -12.626 223.282

orbtensor 20 C
-224.629 -2.045 -31.346
-2.045 -150.069 -0.867
-31.346 -0.867 -60.846
242.323 0.441 13.396
0.441 226.212 0.368
13.396 0.368 223.283

orbtensor 21 H
-10.748 -0.293 -2.867
-0.293 -0.054 -0.079
-2.867 -0.079 -0.687
38.733 0.378 3.800
0.378 24.954 0.104
3.800 0.104 25.669

gtensor (ppt)
-0.125 0.000 0.000
0.000 -0.125 0.000
0.000 0.000 -0.131
-6.329 0.000 0.000
0.000 -6.329 0.000
0.000 0.000 -1.270

zfstensor (cm-1)
-0.765728 -0.000013 -0.000012
-0.000013 -0.765636 -0.000086
-0.000012 -0.000086 0.798978

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	4.4157	-448.18833	-2216.32583	-39.20005	-2255.52588	-2703.71421
2	H	3.0453	25.95567	-402.55442	0.30948	-402.24494	-376.28927
3	C	-0.7137	85.42400	375.09572	1.50991	376.60563	462.02963
4	H	3.0450	25.95600	-402.51036	0.30937	-402.20100	-376.24500
5	C	-0.7127	85.42500	374.57013	1.51017	376.08030	461.50530
6	H	3.0453	25.95600	-402.55442	0.30978	-402.24464	-376.28864
7	C	-0.7120	85.42433	374.21974	1.51086	375.73060	461.15493
8	H	3.0453	25.95533	-402.55442	0.30965	-402.24477	-376.28944
9	C	-0.7123	85.42533	374.39493	1.51105	375.90598	461.33131
10	H	3.0453	25.95567	-402.55442	0.30944	-402.24499	-376.28932
11	C	-0.7133	85.42300	374.92052	1.51068	376.43120	461.85420
12	H	3.0453	25.95567	-402.55442	0.30974	-402.24468	-376.28902
13	C	-0.7130	85.42600	374.74532	1.51025	376.25558	461.68158
14	H	3.0457	25.95600	-402.59849	0.30970	-402.28879	-376.33279
15	C	-0.7123	85.42533	374.39493	1.51077	375.90571	461.33104
16	H	3.0453	25.95567	-402.55442	0.30967	-402.24475	-376.28908
17	C	-0.7130	85.42300	374.74532	1.51074	376.25606	461.67906
18	H	3.0450	25.95600	-402.51036	0.30959	-402.20077	-376.24477
19	C	-0.7130	85.42367	374.74532	1.51084	376.25617	461.67983
20	C	-0.7133	85.42467	374.92052	1.50968	376.43021	461.85487
21	H	3.0443	25.95567	-402.42224	0.30950	-402.11273	-376.15707
13C Average		-0.7129	85.42443	374.67525	1.51050	376.18574	461.61018
1H Average		3.0452	25.95577	-402.53680	0.30959	-402.22721	-376.27144

=====
4VCp2-STO-BP-Pederson
Temperature: 298
Spin: 1.5

atensor 1 V
30.492 0.000 0.000
0.000 30.492 0.004
0.000 0.004 -26.547
-8.141 0.000 0.000
0.000 -8.141 0.000
0.000 0.000 -4.908

atensor 2 H
0.789 -1.392 -1.265
-1.392 4.207 3.558
-1.265 3.558 4.124
0.013 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

atensor 3 C
-1.711 -0.244 -0.593
-0.244 -1.112 1.667
-0.593 1.667 0.606
0.046 0.006 0.007
0.006 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H
4.699 0.121 -3.775
0.121 0.297 -0.104
-3.775 -0.104 4.123
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C
-1.024 0.021 -1.769

0.021 -1.797 -0.049
-1.769 -0.049 0.607
0.028 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.646 1.196 -1.068
1.196 4.350 -3.622
-1.068 -3.622 4.124
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.735 0.210 -0.501
0.210 -1.085 -1.698
-0.501 -1.698 0.608
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.293 -2.056 3.115
-2.056 1.703 -2.135
3.115 -2.135 4.124
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.271 -0.361 1.460
-0.361 -1.550 -1.001
1.460 -1.001 0.608
0.034 0.010 -0.016
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.063 2.130 2.993
2.130 1.933 2.303
2.993 2.303 4.124
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.312 0.374 1.403
0.374 -1.511 1.079
1.403 1.079 0.607
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.016 -0.013 0.000

atensor 12 H
0.646 1.196 1.068
1.196 4.349 3.622
1.068 3.622 4.125
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.736 0.210 0.501
0.210 -1.086 1.698
0.501 1.698 0.607
0.047 -0.006 -0.006

-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.293 -2.056 -3.115
-2.056 1.703 2.135
-3.115 2.135 4.125
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.271 -0.361 -1.460
-0.361 -1.550 1.001
-1.460 1.000 0.608
0.034 0.010 0.016
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.063 2.131 -2.993
2.131 1.933 -2.303
-2.993 -2.303 4.124
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.312 0.374 -1.403
0.374 -1.510 -1.079
-1.403 -1.079 0.607
0.035 -0.010 0.016
-0.010 0.041 0.012
0.016 0.013 0.000

atensor 18 H
0.788 -1.392 1.265
-1.392 4.208 -3.558
1.265 -3.558 4.123
0.013 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.711 -0.244 0.593
-0.244 -1.111 -1.668
0.593 -1.668 0.607
0.046 0.006 -0.007
0.006 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.025 0.021 1.769
0.021 -1.797 0.048
1.769 0.048 0.606
0.028 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.698 0.121 3.775
0.121 0.296 0.103
3.775 0.103 4.123
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3063.695 -0.014 -0.020
-0.014 -3063.683 -0.148
-0.020 -0.148 -351.484
1708.729 0.000 0.000
0.000 1708.729 -0.001
0.000 -0.001 1716.839

orbtensor 2 H
-1.248 3.381 0.961
3.381 -9.554 -2.702
0.961 -2.702 -0.687
26.492 -4.356 -1.274
-4.356 37.194 3.582
-1.274 3.582 25.670

orbtensor 3 C
-158.398 23.568 10.503
23.568 -216.303 -29.554
10.503 -29.554 -60.849
228.012 -5.093 -4.490
-5.093 240.524 12.628
-4.490 12.628 223.286

orbtensor 4 H
-10.748 -0.294 2.866
-0.294 -0.054 0.079
2.866 0.079 -0.686
38.733 0.379 -3.800
0.379 24.954 -0.104
-3.800 -0.104 25.669

orbtensor 5 C
-224.630 -2.048 31.345
-2.048 -150.070 0.857
31.345 0.857 -60.845
242.324 0.443 -13.396
0.443 226.213 -0.368
-13.396 -0.368 223.283

orbtensor 6 H
-0.904 -2.905 0.811
-2.905 -9.899 2.751
0.811 2.751 -0.686
26.048 3.744 -1.075
3.744 37.640 -3.646
-1.075 -3.646 25.669

orbtensor 7 C
-155.990 -20.258 8.866
-20.258 -218.715 30.079
8.866 30.079 -60.846
227.493 4.378 -3.790
4.378 241.048 -12.854
-3.790 -12.854 223.283

orbtensor 8 H
-7.333 4.994 -2.366
4.994 -3.470 1.622
-2.366 1.622 -0.687
34.332 -6.435 3.136
-6.435 29.355 -2.150
3.136 -2.150 25.669

orbtensor 9 C
-200.816 34.822 -25.874
34.822 -173.885 17.732

-25.874	17.732	-60.848
237.180	-7.524	11.055
-7.524	231.361	-7.577
11.055	-7.577	223.284

orbtensor 10 H

-6.774	-5.176	-2.274
-5.176	-4.028	-1.749
-2.274	-1.749	-0.687
33.612	6.669	3.014
6.669	30.074	2.318
3.014	2.318	25.670

orbtensor 11 C

-196.923	-36.084	-24.865
-36.084	-177.780	-19.129
-24.865	-19.129	-60.850
236.337	7.797	10.623
7.797	232.200	8.172
10.623	8.172	223.285

orbtensor 12 H

-0.903	-2.905	-0.811
-2.905	-9.899	-2.751
-0.811	-2.751	-0.687
26.047	3.743	1.075
3.743	37.639	3.647
1.075	3.647	25.670

orbtensor 13 C

-155.986	-20.258	-8.868
-20.258	-218.707	-30.094
-8.868	-30.094	-60.852
227.493	4.377	3.790
4.377	241.043	12.856
3.790	12.856	223.287

orbtensor 14 H

-7.332	4.994	2.366
4.994	-3.469	-1.622
2.366	-1.622	-0.687
34.332	-6.435	-3.136
-6.435	29.354	2.150
-3.136	2.150	25.670

orbtensor 15 C

-200.816	34.818	25.874
34.818	-173.880	-17.742
25.874	-17.742	-60.852
237.179	-7.522	-11.055
-7.522	231.358	7.577
-11.055	7.577	223.287

orbtensor 16 H

-6.774	-5.176	2.273
-5.176	-4.029	1.749
2.273	1.749	-0.687
33.613	6.669	-3.013
6.669	30.075	-2.318
-3.013	-2.318	25.669

orbtensor 17 C

-196.924	-36.087	24.857
-36.087	-177.785	19.114
24.857	19.114	-60.844
236.337	7.798	-10.622
7.798	232.202	-8.171

-10.622 -8.171 223.283

orbtensor 18 H

-1.248 3.381 -0.960
3.381 -9.554 2.701
-0.960 2.701 -0.686
26.492 -4.356 1.273
-4.356 37.195 -3.581
1.273 -3.581 25.669

orbtensor 19 C

-158.399 23.568 -10.502
23.568 -216.310 29.537
-10.502 29.537 -60.842
228.013 -5.093 4.489
-5.093 240.527 -12.626
4.489 -12.626 223.282

orbtensor 20 C

-224.629 -2.045 -31.346
-2.045 -150.069 -0.867
-31.346 -0.867 -60.846
242.323 0.441 13.396
0.441 226.212 0.368
13.396 0.368 223.283

orbtensor 21 H

-10.748 -0.293 -2.867
-0.293 -0.054 -0.079
-2.867 -0.079 -0.687
38.733 0.378 3.800
0.378 24.954 0.104
3.800 0.104 25.669

gtensor (ppt)

-0.125 0.000 0.000
0.000 -0.125 0.000
0.000 0.000 -0.131
-6.329 0.000 0.000
0.000 -6.329 0.000
0.000 0.000 -1.270

zfstensor (cm-1)

-0.294419 0.000000 -0.000006
0.000000 -0.294419 0.000048
-0.000006 0.000048 0.588838

averaging

13C Average:3,5,7,9,11,13,15,17,19,20

1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	4.4157	-448.18833	-2216.34223	-15.53436	-2231.87659	-2680.06492
2	H	3.0453	25.95567	-402.55740	0.12277	-402.43463	-376.47896
3	C	-0.7137	85.42400	375.09849	0.59862	375.69711	461.12111
4	H	3.0450	25.95600	-402.51334	0.12262	-402.39072	-376.43472
5	C	-0.7127	85.42500	374.57290	0.59847	375.17137	460.59637
6	H	3.0453	25.95600	-402.55740	0.12260	-402.43481	-376.47881
7	C	-0.7120	85.42433	374.22250	0.59844	374.82095	460.24528
8	H	3.0453	25.95533	-402.55740	0.12262	-402.43478	-376.47945
9	C	-0.7123	85.42533	374.39770	0.59864	374.99634	460.42167
10	H	3.0453	25.95567	-402.55740	0.12273	-402.43467	-376.47901
11	C	-0.7133	85.42300	374.92330	0.59884	375.52213	460.94513
12	H	3.0453	25.95567	-402.55740	0.12288	-402.43452	-376.47885

13	C	-0.7130	85.42600	374.74810	0.59876	375.34686	460.77286
14	H	3.0457	25.95600	-402.60147	0.12282	-402.47865	-376.52265
15	C	-0.7123	85.42533	374.39770	0.59887	374.99657	460.42190
16	H	3.0453	25.95567	-402.55740	0.12264	-402.43477	-376.47910
17	C	-0.7130	85.42300	374.74810	0.59851	375.34661	460.76961
18	H	3.0450	25.95600	-402.51334	0.12252	-402.39082	-376.43482
19	C	-0.7130	85.42367	374.74810	0.59843	375.34653	460.77020
20	C	-0.7133	85.42467	374.92330	0.59828	375.52158	460.94624
21	H	3.0443	25.95567	-402.42521	0.12267	-402.30254	-376.34687
13C Average		-0.7129	85.42443	374.67802	0.59859	375.27660	460.70104
1H Average		3.0452	25.95577	-402.53978	0.12269	-402.41709	-376.46132

=====
 4VCp2-STO-BP-Van-Wullen

Temperature: 298

Spin: 1.5

atensor 1 V

30.492 0.000 0.000
 0.000 30.492 0.004
 0.000 0.004 -26.547
 -8.141 0.000 0.000
 0.000 -8.141 0.000
 0.000 0.000 -4.908

atensor 2 H

0.789 -1.392 -1.265
 -1.392 4.207 3.558
 -1.265 3.558 4.124
 0.013 0.003 0.007
 0.003 0.006 -0.020
 0.004 -0.011 -0.003

atensor 3 C

-1.711 -0.244 -0.593
 -0.244 -1.112 1.667
 -0.593 1.667 0.606
 0.046 0.006 0.007
 0.006 0.030 -0.019
 0.007 -0.020 0.000

atensor 4 H

4.699 0.121 -3.775
 0.121 0.297 -0.104
 -3.775 -0.104 4.123
 0.004 0.000 0.021
 0.000 0.015 0.001
 0.012 0.000 -0.003

atensor 5 C

-1.024 0.021 -1.769
 0.021 -1.797 -0.049
 -1.769 -0.049 0.607
 0.028 -0.001 0.020
 -0.001 0.048 0.001
 0.021 0.001 0.000

atensor 6 H

0.646 1.196 -1.068
 1.196 4.350 -3.622
 -1.068 -3.622 4.124
 0.014 -0.003 0.006
 -0.003 0.005 0.020
 0.003 0.011 -0.003

atensor 7 C

-1.735 0.210 -0.501
0.210 -1.085 -1.698
-0.501 -1.698 0.608
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.293 -2.056 3.115
-2.056 1.703 -2.135
3.115 -2.135 4.124
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.271 -0.361 1.460
-0.361 -1.550 -1.001
1.460 -1.001 0.608
0.034 0.010 -0.016
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.063 2.130 2.993
2.130 1.933 2.303
2.993 2.303 4.124
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.312 0.374 1.403
0.374 -1.511 1.079
1.403 1.079 0.607
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.016 -0.013 0.000

atensor 12 H
0.646 1.196 1.068
1.196 4.349 3.622
1.068 3.622 4.125
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.736 0.210 0.501
0.210 -1.086 1.698
0.501 1.698 0.607
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.293 -2.056 -3.115
-2.056 1.703 2.135
-3.115 2.135 4.125
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.271 -0.361 -1.460
-0.361 -1.550 1.001
-1.460 1.000 0.608

0.034 0.010 0.016
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.063 2.131 -2.993
2.131 1.933 -2.303
-2.993 -2.303 4.124
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.312 0.374 -1.403
0.374 -1.510 -1.079
-1.403 -1.079 0.607
0.035 -0.010 0.016
-0.010 0.041 0.012
0.016 0.013 0.000

atensor 18 H
0.788 -1.392 1.265
-1.392 4.208 -3.558
1.265 -3.558 4.123
0.013 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.711 -0.244 0.593
-0.244 -1.111 -1.668
0.593 -1.668 0.607
0.046 0.006 -0.007
0.006 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.025 0.021 1.769
0.021 -1.797 0.048
1.769 0.048 0.606
0.028 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.698 0.121 3.775
0.121 0.296 0.103
3.775 0.103 4.123
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3063.695 -0.014 -0.020
-0.014 -3063.683 -0.148
-0.020 -0.148 -351.484
1708.729 0.000 0.000
0.000 1708.729 -0.001
0.000 -0.001 1716.839

orbtensor 2 H
-1.248 3.381 0.961
3.381 -9.554 -2.702
0.961 -2.702 -0.687
26.492 -4.356 -1.274
-4.356 37.194 3.582
-1.274 3.582 25.670

orbtensor 3 C
-158.398 23.568 10.503
23.568 -216.303 -29.554
10.503 -29.554 -60.849
228.012 -5.093 -4.490
-5.093 240.524 12.628
-4.490 12.628 223.286

orbtensor 4 H
-10.748 -0.294 2.866
-0.294 -0.054 0.079
2.866 0.079 -0.686
38.733 0.379 -3.800
0.379 24.954 -0.104
-3.800 -0.104 25.669

orbtensor 5 C
-224.630 -2.048 31.345
-2.048 -150.070 0.857
31.345 0.857 -60.845
242.324 0.443 -13.396
0.443 226.213 -0.368
-13.396 -0.368 223.283

orbtensor 6 H
-0.904 -2.905 0.811
-2.905 -9.899 2.751
0.811 2.751 -0.686
26.048 3.744 -1.075
3.744 37.640 -3.646
-1.075 -3.646 25.669

orbtensor 7 C
-155.990 -20.258 8.866
-20.258 -218.715 30.079
8.866 30.079 -60.846
227.493 4.378 -3.790
4.378 241.048 -12.854
-3.790 -12.854 223.283

orbtensor 8 H
-7.333 4.994 -2.366
4.994 -3.470 1.622
-2.366 1.622 -0.687
34.332 -6.435 3.136
-6.435 29.355 -2.150
3.136 -2.150 25.669

orbtensor 9 C
-200.816 34.822 -25.874
34.822 -173.885 17.732
-25.874 17.732 -60.848
237.180 -7.524 11.055
-7.524 231.361 -7.577
11.055 -7.577 223.284

orbtensor 10 H
-6.774 -5.176 -2.274
-5.176 -4.028 -1.749
-2.274 -1.749 -0.687
33.612 6.669 3.014
6.669 30.074 2.318
3.014 2.318 25.670

orbtensor 11 C
-196.923 -36.084 -24.865

-36.084	-177.780	-19.129
-24.865	-19.129	-60.850
236.337	7.797	10.623
7.797	232.200	8.172
10.623	8.172	223.285

orbtensor 12 H

-0.903	-2.905	-0.811
-2.905	-9.899	-2.751
-0.811	-2.751	-0.687
26.047	3.743	1.075
3.743	37.639	3.647
1.075	3.647	25.670

orbtensor 13 C

-155.986	-20.258	-8.868
-20.258	-218.707	-30.094
-8.868	-30.094	-60.852
227.493	4.377	3.790
4.377	241.043	12.856
3.790	12.856	223.287

orbtensor 14 H

-7.332	4.994	2.366
4.994	-3.469	-1.622
2.366	-1.622	-0.687
34.332	-6.435	-3.136
-6.435	29.354	2.150
-3.136	2.150	25.670

orbtensor 15 C

-200.816	34.818	25.874
34.818	-173.880	-17.742
25.874	-17.742	-60.852
237.179	-7.522	-11.055
-7.522	231.358	7.577
-11.055	7.577	223.287

orbtensor 16 H

-6.774	-5.176	2.273
-5.176	-4.029	1.749
2.273	1.749	-0.687
33.613	6.669	-3.013
6.669	30.075	-2.318
-3.013	-2.318	25.669

orbtensor 17 C

-196.924	-36.087	24.857
-36.087	-177.785	19.114
24.857	19.114	-60.844
236.337	7.798	-10.622
7.798	232.202	-8.171
-10.622	-8.171	223.283

orbtensor 18 H

-1.248	3.381	-0.960
3.381	-9.554	2.701
-0.960	2.701	-0.686
26.492	-4.356	1.273
-4.356	37.195	-3.581
1.273	-3.581	25.669

orbtensor 19 C

-158.399	23.568	-10.502
23.568	-216.310	29.537
-10.502	29.537	-60.842
228.013	-5.093	4.489

-5.093 240.527 -12.626
 4.489 -12.626 223.282

orbtensor 20 C
 -224.629 -2.045 -31.346
 -2.045 -150.069 -0.867
 -31.346 -0.867 -60.846
 242.323 0.441 13.396
 0.441 226.212 0.368
 13.396 0.368 223.283

orbtensor 21 H
 -10.748 -0.293 -2.867
 -0.293 -0.054 -0.079
 -2.867 -0.079 -0.687
 38.733 0.378 3.800
 0.378 24.954 0.104
 3.800 0.104 25.669

gtensor (ppt)
 -0.125 0.000 0.000
 0.000 -0.125 0.000
 0.000 0.000 -0.131
 -6.329 0.000 0.000
 0.000 -6.329 0.000
 0.000 0.000 -1.270

zfstensor (cm-1)
 -0.441628 0.000000 -0.000009
 0.000000 -0.441629 0.000072
 -0.000009 0.000072 0.883257

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	4.4157	-448.18833	-2216.33233	-30.87555	-2247.20788	-2695.39621
2	H	3.0453	25.95567	-402.55561	0.24398	-402.31163	-376.35596
3	C	-0.7137	85.42400	375.09682	1.18971	376.28653	461.71053
4	H	3.0450	25.95600	-402.51154	0.24370	-402.26784	-376.31184
5	C	-0.7127	85.42500	374.57123	1.18948	375.76071	461.18571
6	H	3.0453	25.95600	-402.55561	0.24371	-402.31189	-376.35589
7	C	-0.7120	85.42433	374.22083	1.18952	375.41035	460.83469
8	H	3.0453	25.95533	-402.55561	0.24375	-402.31186	-376.35652
9	C	-0.7123	85.42533	374.39603	1.18989	375.58592	461.01125
10	H	3.0453	25.95567	-402.55561	0.24391	-402.31169	-376.35603
11	C	-0.7133	85.42300	374.92162	1.19019	376.11181	461.53481
12	H	3.0453	25.95567	-402.55561	0.24419	-402.31141	-376.35574
13	C	-0.7130	85.42600	374.74642	1.18999	375.93642	461.36242
14	H	3.0457	25.95600	-402.59967	0.24408	-402.35558	-376.39958
15	C	-0.7123	85.42533	374.39603	1.19023	375.58626	461.01159
16	H	3.0453	25.95567	-402.55561	0.24377	-402.31184	-376.35617
17	C	-0.7130	85.42300	374.74642	1.18963	375.93605	461.35905
18	H	3.0450	25.95600	-402.51154	0.24355	-402.26799	-376.31199
19	C	-0.7130	85.42367	374.74642	1.18951	375.93593	461.35960
20	C	-0.7133	85.42467	374.92162	1.18913	376.11075	461.53542
21	H	3.0443	25.95567	-402.42342	0.24383	-402.17959	-376.22392
13C Average		-0.7129	85.42443	374.67634	1.18973	375.86607	461.29051
1H Average		3.0452	25.95577	-402.53798	0.24385	-402.29413	-376.33837

4VCp2-STO-PBE-No-ZFS

Temperature: 298
Spin: 1.5

atensor 1 V
27.854 0.000 0.000
0.000 27.853 0.004
0.000 0.004 -28.684
-8.154 0.000 0.000
0.000 -8.154 0.000
0.000 0.000 -4.851

atensor 2 H
0.771 -1.406 -1.261
-1.406 4.225 3.546
-1.261 3.546 4.112
0.014 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

atensor 3 C
-1.743 -0.247 -0.589
-0.247 -1.136 1.656
-0.589 1.656 0.708
0.046 0.007 0.007
0.007 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H
4.721 0.122 -3.762
0.122 0.275 -0.103
-3.762 -0.103 4.112
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C
-1.049 0.022 -1.757
0.022 -1.831 -0.048
-1.757 -0.048 0.707
0.027 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.628 1.208 -1.065
1.208 4.369 -3.610
-1.065 -3.610 4.112
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.770 0.212 -0.497
0.212 -1.112 -1.686
-0.497 -1.686 0.707
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.301 -2.077 3.104
-2.077 1.695 -2.128
3.104 -2.128 4.112
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.299 -0.365 1.449
-0.365 -1.581 -0.994
1.449 -0.994 0.708
0.034 0.010 -0.017
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.069 2.152 2.983
2.152 1.927 2.295
2.983 2.295 4.113
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.340 0.378 1.393
0.378 -1.540 1.071
1.393 1.071 0.708
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.017 -0.013 0.000

atensor 12 H
0.627 1.208 1.065
1.208 4.368 3.610
1.065 3.610 4.112
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.769 0.212 0.497
0.212 -1.111 1.686
0.497 1.686 0.709
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.301 -2.076 -3.105
-2.076 1.695 2.128
-3.105 2.128 4.113
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.299 -0.365 -1.450
-0.365 -1.581 0.993
-1.450 0.993 0.709
0.034 0.010 0.017
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.069 2.152 -2.983
2.152 1.928 -2.295
-2.983 -2.295 4.112
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.340 0.378 -1.393
0.378 -1.540 -1.072

-1.393 -1.072 0.708
0.035 -0.010 0.016
-0.010 0.041 0.012
0.017 0.013 0.000

atensor 18 H
0.771 -1.406 1.261
-1.406 4.225 -3.546
1.261 -3.546 4.111
0.014 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.744 -0.247 0.589
-0.247 -1.136 -1.656
0.589 -1.656 0.707
0.046 0.007 -0.007
0.007 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.049 0.021 1.757
0.021 -1.831 0.048
1.757 0.048 0.708
0.027 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.721 0.122 3.762
0.122 0.274 0.103
3.762 0.103 4.111
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3088.084 -0.002 -0.019
-0.002 -3088.085 -0.146
-0.019 -0.146 -354.934
1709.344 0.000 0.000
0.000 1709.344 0.000
0.000 0.000 1715.988

orbtensor 2 H
-1.061 3.360 0.966
3.360 -9.316 -2.719
0.966 -2.719 -0.665
26.274 -4.309 -1.273
-4.309 36.860 3.581
-1.273 3.581 25.573

orbtensor 3 C
-155.939 23.789 10.753
23.789 -214.384 -30.260
10.753 -30.260 -59.550
226.307 -5.220 -4.702
-5.220 239.130 13.226
-4.702 13.226 222.717

orbtensor 4 H
-10.502 -0.292 2.884
-0.292 0.126 0.079
2.884 0.079 -0.665
38.381 0.375 -3.799
0.375 24.751 -0.104

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-3.799   -0.104   25.572

orbtensor 5 C
-222.791  -2.067   32.095
-2.067  -147.533   0.878
32.095   0.878  -59.545
240.973   0.454  -14.032
0.454  224.459  -0.385
-14.032  -0.385  222.714

orbtensor 6 H
-0.717  -2.888   0.816
-2.888  -9.658   2.768
0.816   2.768  -0.664
25.833   3.703  -1.075
3.703  37.300  -3.646
-1.075  -3.646  25.572

orbtensor 7 C
-153.505  -20.448   9.077
-20.448  -216.819  30.797
9.077   30.797  -59.545
225.769   4.487  -3.970
4.487  239.663  -13.465
-3.970  -13.465  222.714

orbtensor 8 H
-7.107   4.964  -2.380
4.964  -3.269   1.632
-2.380   1.632  -0.665
34.028  -6.366   3.136
-6.366  29.105  -2.149
3.136  -2.149  25.572

orbtensor 9 C
-198.752   35.148  -26.493
35.148  -171.571  18.154
-26.493  18.154  -59.549
235.698  -7.712  11.580
-7.712  229.735  -7.937
11.580  -7.937  222.716

orbtensor 10 H
-6.553  -5.144  -2.287
-5.144  -3.824  -1.760
-2.287  -1.760  -0.665
33.317   6.597   3.013
6.597  29.817   2.318
3.013   2.318  25.573

orbtensor 11 C
-194.823  -36.421  -25.458
-36.421  -175.500  -19.586
-25.458  -19.586  -59.552
234.839   7.991  11.126
7.991  230.599   8.560
11.126   8.560  222.718

orbtensor 12 H
-0.718  -2.887  -0.816
-2.887  -9.659  -2.768
-0.816  -2.768  -0.665
25.834   3.703   1.075
3.703  37.300   3.646
1.075   3.646  25.573

orbtensor 13 C

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-153.509	-20.445	-9.081
-20.445	-216.812	-30.813
-9.081	-30.813	-59.553
225.774	4.486	3.970
4.486	239.663	13.465
3.970	13.465	222.718

orbtensor 14 H

-7.108	4.963	2.380
4.963	-3.268	-1.632
2.380	-1.632	-0.665
34.029	-6.365	-3.136
-6.365	29.105	2.149
-3.136	2.149	25.573

orbtensor 15 C

-198.755	35.142	26.493
35.142	-171.568	-18.165
26.493	-18.165	-59.553
235.701	-7.710	-11.579
-7.710	229.735	7.937
-11.579	7.937	222.718

orbtensor 16 H

-6.553	-5.144	2.286
-5.144	-3.824	1.759
2.286	1.759	-0.665
33.317	6.597	-3.012
6.597	29.817	-2.317
-3.012	-2.317	25.572

orbtensor 17 C

-194.822	-36.426	25.450
-36.426	-175.505	19.570
25.450	19.570	-59.546
234.837	7.993	-11.125
7.993	230.600	-8.559
-11.125	-8.559	222.715

orbtensor 18 H

-1.061	3.360	-0.966
3.360	-9.316	2.718
-0.966	2.718	-0.664
26.273	-4.309	1.273
-4.309	36.860	-3.580
1.273	-3.580	25.572

orbtensor 19 C

-155.936	23.791	-10.752
23.791	-214.393	30.243
-10.752	30.243	-59.542
226.304	-5.220	4.702
-5.220	239.132	-13.225
4.702	-13.225	222.713

orbtensor 20 C

-222.791	-2.063	-32.094
-2.063	-147.536	-0.888
-32.094	-0.888	-59.548
240.975	0.452	14.031
0.452	224.462	0.385
14.031	0.385	222.715

orbtensor 21 H

-10.503	-0.291	-2.884
-0.291	0.125	-0.079
-2.884	-0.079	-0.665

```

38.382    0.374    3.799
0.374    24.752    0.104
3.799    0.104    25.572

```

```

gtensor (ppt)
-0.126    0.000    0.000
0.000    -0.126    0.000
0.000    0.000    -0.132
-6.413    0.000    0.000
0.000    -6.413    0.000
0.000    0.000    -1.286

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	1.9547	-465.47567	-981.07452	15.22231	-965.85220	-1431.32787
2	H	3.0417	25.88833	-402.06230	-0.12057	-402.18286	-376.29453
3	C	-0.6983	86.09367	367.02989	-0.63165	366.39824	452.49190
4	H	3.0413	25.88767	-402.01824	-0.12061	-402.13884	-376.25117
5	C	-0.6993	86.09233	367.55547	-0.63165	366.92382	453.01615
6	H	3.0417	25.88867	-402.06230	-0.12057	-402.18286	-376.29420
7	C	-0.6997	86.09233	367.73066	-0.63180	367.09886	453.19119
8	H	3.0413	25.88800	-402.01824	-0.12061	-402.13884	-376.25084
9	C	-0.6987	86.09233	367.20508	-0.63180	366.57328	452.66561
10	H	3.0417	25.88833	-402.06230	-0.12068	-402.18298	-376.29464
11	C	-0.6987	86.09367	367.20508	-0.63180	366.57328	452.66695
12	H	3.0410	25.88833	-401.97417	-0.12064	-402.09482	-376.20648
13	C	-0.6983	86.09367	367.02989	-0.63210	366.39779	452.49145
14	H	3.0417	25.88867	-402.06230	-0.12068	-402.18298	-376.29431
15	C	-0.6983	86.09267	367.02989	-0.63210	366.39779	452.49045
16	H	3.0417	25.88800	-402.06230	-0.12057	-402.18286	-376.29486
17	C	-0.6987	86.09300	367.20508	-0.63180	366.57328	452.66628
18	H	3.0413	25.88800	-402.01824	-0.12049	-402.13873	-376.25073
19	C	-0.6990	86.09267	367.38027	-0.63150	366.74877	452.84144
20	C	-0.6990	86.09233	367.38027	-0.63195	366.74832	452.84066
21	H	3.0407	25.88767	-401.93011	-0.12057	-402.05068	-376.16301
13C Average		-0.6988	86.09287	367.27516	-0.63181	366.64334	452.73621
1H Average		3.0414	25.88817	-402.02705	-0.12060	-402.14765	-376.25948

```

=====
4VCp2-STO-PBE-Neese
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
27.854 0.000 0.000
0.000 27.853 0.004
0.000 0.004 -28.684
-8.154 0.000 0.000
0.000 -8.154 0.000
0.000 0.000 -4.851

```

```

atensor 2 H
0.771 -1.406 -1.261
-1.406 4.225 3.546
-1.261 3.546 4.112
0.014 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

```

```

atensor 3 C

```

-1.743 -0.247 -0.589
-0.247 -1.136 1.656
-0.589 1.656 0.708
0.046 0.007 0.007
0.007 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H
4.721 0.122 -3.762
0.122 0.275 -0.103
-3.762 -0.103 4.112
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C
-1.049 0.022 -1.757
0.022 -1.831 -0.048
-1.757 -0.048 0.707
0.027 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.628 1.208 -1.065
1.208 4.369 -3.610
-1.065 -3.610 4.112
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.770 0.212 -0.497
0.212 -1.112 -1.686
-0.497 -1.686 0.707
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.301 -2.077 3.104
-2.077 1.695 -2.128
3.104 -2.128 4.112
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.299 -0.365 1.449
-0.365 -1.581 -0.994
1.449 -0.994 0.708
0.034 0.010 -0.017
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.069 2.152 2.983
2.152 1.927 2.295
2.983 2.295 4.113
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.340 0.378 1.393
0.378 -1.540 1.071
1.393 1.071 0.708

0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.017 -0.013 0.000

atensor 12 H
0.627 1.208 1.065
1.208 4.368 3.610
1.065 3.610 4.112
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.769 0.212 0.497
0.212 -1.111 1.686
0.497 1.686 0.709
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.301 -2.076 -3.105
-2.076 1.695 2.128
-3.105 2.128 4.113
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.299 -0.365 -1.450
-0.365 -1.581 0.993
-1.450 0.993 0.709
0.034 0.010 0.017
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.069 2.152 -2.983
2.152 1.928 -2.295
-2.983 -2.295 4.112
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.340 0.378 -1.393
0.378 -1.540 -1.072
-1.393 -1.072 0.708
0.035 -0.010 0.016
-0.010 0.041 0.012
0.017 0.013 0.000

atensor 18 H
0.771 -1.406 1.261
-1.406 4.225 -3.546
1.261 -3.546 4.111
0.014 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.744 -0.247 0.589
-0.247 -1.136 -1.656
0.589 -1.656 0.707
0.046 0.007 -0.007
0.007 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.049 0.021 1.757
0.021 -1.831 0.048
1.757 0.048 0.708
0.027 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.721 0.122 3.762
0.122 0.274 0.103
3.762 0.103 4.111
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3088.084 -0.002 -0.019
-0.002 -3088.085 -0.146
-0.019 -0.146 -354.934
1709.344 0.000 0.000
0.000 1709.344 0.000
0.000 0.000 1715.988

orbtensor 2 H
-1.061 3.360 0.966
3.360 -9.316 -2.719
0.966 -2.719 -0.665
26.274 -4.309 -1.273
-4.309 36.860 3.581
-1.273 3.581 25.573

orbtensor 3 C
-155.939 23.789 10.753
23.789 -214.384 -30.260
10.753 -30.260 -59.550
226.307 -5.220 -4.702
-5.220 239.130 13.226
-4.702 13.226 222.717

orbtensor 4 H
-10.502 -0.292 2.884
-0.292 0.126 0.079
2.884 0.079 -0.665
38.381 0.375 -3.799
0.375 24.751 -0.104
-3.799 -0.104 25.572

orbtensor 5 C
-222.791 -2.067 32.095
-2.067 -147.533 0.878
32.095 0.878 -59.545
240.973 0.454 -14.032
0.454 224.459 -0.385
-14.032 -0.385 222.714

orbtensor 6 H
-0.717 -2.888 0.816
-2.888 -9.658 2.768
0.816 2.768 -0.664
25.833 3.703 -1.075
3.703 37.300 -3.646
-1.075 -3.646 25.572

orbtensor 7 C
-153.505 -20.448 9.077

-20.448	-216.819	30.797
9.077	30.797	-59.545
225.769	4.487	-3.970
4.487	239.663	-13.465
-3.970	-13.465	222.714

orbtensor 8 H

-7.107	4.964	-2.380
4.964	-3.269	1.632
-2.380	1.632	-0.665
34.028	-6.366	3.136
-6.366	29.105	-2.149
3.136	-2.149	25.572

orbtensor 9 C

-198.752	35.148	-26.493
35.148	-171.571	18.154
-26.493	18.154	-59.549
235.698	-7.712	11.580
-7.712	229.735	-7.937
11.580	-7.937	222.716

orbtensor 10 H

-6.553	-5.144	-2.287
-5.144	-3.824	-1.760
-2.287	-1.760	-0.665
33.317	6.597	3.013
6.597	29.817	2.318
3.013	2.318	25.573

orbtensor 11 C

-194.823	-36.421	-25.458
-36.421	-175.500	-19.586
-25.458	-19.586	-59.552
234.839	7.991	11.126
7.991	230.599	8.560
11.126	8.560	222.718

orbtensor 12 H

-0.718	-2.887	-0.816
-2.887	-9.659	-2.768
-0.816	-2.768	-0.665
25.834	3.703	1.075
3.703	37.300	3.646
1.075	3.646	25.573

orbtensor 13 C

-153.509	-20.445	-9.081
-20.445	-216.812	-30.813
-9.081	-30.813	-59.553
225.774	4.486	3.970
4.486	239.663	13.465
3.970	13.465	222.718

orbtensor 14 H

-7.108	4.963	2.380
4.963	-3.268	-1.632
2.380	-1.632	-0.665
34.029	-6.365	-3.136
-6.365	29.105	2.149
-3.136	2.149	25.573

orbtensor 15 C

-198.755	35.142	26.493
35.142	-171.568	-18.165
26.493	-18.165	-59.553
235.701	-7.710	-11.579

-7.710 229.735 7.937
-11.579 7.937 222.718

orbtensor 16 H
-6.553 -5.144 2.286
-5.144 -3.824 1.759
2.286 1.759 -0.665
33.317 6.597 -3.012
6.597 29.817 -2.317
-3.012 -2.317 25.572

orbtensor 17 C
-194.822 -36.426 25.450
-36.426 -175.505 19.570
25.450 19.570 -59.546
234.837 7.993 -11.125
7.993 230.600 -8.559
-11.125 -8.559 222.715

orbtensor 18 H
-1.061 3.360 -0.966
3.360 -9.316 2.718
-0.966 2.718 -0.664
26.273 -4.309 1.273
-4.309 36.860 -3.580
1.273 -3.580 25.572

orbtensor 19 C
-155.936 23.791 -10.752
23.791 -214.393 30.243
-10.752 30.243 -59.542
226.304 -5.220 4.702
-5.220 239.132 -13.225
4.702 -13.225 222.713

orbtensor 20 C
-222.791 -2.063 -32.094
-2.063 -147.536 -0.888
-32.094 -0.888 -59.548
240.975 0.452 14.031
0.452 224.462 0.385
14.031 0.385 222.715

orbtensor 21 H
-10.503 -0.291 -2.884
-0.291 0.125 -0.079
-2.884 -0.079 -0.665
38.382 0.374 3.799
0.374 24.752 0.104
3.799 0.104 25.572

gtensor (ppt)
-0.126 0.000 0.000
0.000 -0.126 0.000
0.000 0.000 -0.132
-6.413 0.000 0.000
0.000 -6.413 0.000
0.000 0.000 -1.286

zfstensor (cm-1)
-0.318632 0.947878 -0.000002
-0.947878 -0.318632 0.000061
0.000057 0.000022 1.000000

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	1.9547	-465.47567	-981.06495	-30.12973	-1011.19468	-1476.67034
2	H	3.0417	25.88833	-402.05838	0.23870	-401.81968	-375.93134
3	C	-0.6983	86.09367	367.02631	1.25034	368.27664	454.37031
4	H	3.0413	25.88767	-402.01431	0.23866	-401.77565	-375.88799
5	C	-0.6993	86.09233	367.55188	1.25013	368.80201	454.89435
6	H	3.0417	25.88867	-402.05838	0.23855	-401.81983	-375.93116
7	C	-0.6997	86.09233	367.72707	1.25036	368.97743	455.06977
8	H	3.0413	25.88800	-402.01431	0.23871	-401.77560	-375.88760
9	C	-0.6987	86.09233	367.20150	1.25053	368.45202	454.54436
10	H	3.0417	25.88833	-402.05838	0.23896	-401.81942	-375.93109
11	C	-0.6987	86.09367	367.20150	1.25070	368.45219	454.54586
12	H	3.0410	25.88833	-401.97025	0.23888	-401.73137	-375.84304
13	C	-0.6983	86.09367	367.02631	1.25129	368.27760	454.37126
14	H	3.0417	25.88867	-402.05838	0.23887	-401.81951	-375.93084
15	C	-0.6983	86.09267	367.02631	1.25112	368.27743	454.37010
16	H	3.0417	25.88800	-402.05838	0.23855	-401.81982	-375.93182
17	C	-0.6987	86.09300	367.20150	1.25036	368.45186	454.54486
18	H	3.0413	25.88800	-402.01431	0.23844	-401.77588	-375.88788
19	C	-0.6990	86.09267	367.37669	1.24983	368.62652	454.71919
20	C	-0.6990	86.09233	367.37669	1.25093	368.62762	454.71995
21	H	3.0407	25.88767	-401.92619	0.23870	-401.68750	-375.79983
13C Average		-0.6988	86.09287	367.27157	1.25056	368.52213	454.61500
1H Average		3.0414	25.88817	-402.02313	0.23870	-401.78443	-375.89626

=====
 4VCp2-STO-PBE-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 V
 27.854 0.000 0.000
 0.000 27.853 0.004
 0.000 0.004 -28.684
 -8.154 0.000 0.000
 0.000 -8.154 0.000
 0.000 0.000 -4.851

atensor 2 H
 0.771 -1.406 -1.261
 -1.406 4.225 3.546
 -1.261 3.546 4.112
 0.014 0.003 0.007
 0.003 0.006 -0.020
 0.004 -0.011 -0.003

atensor 3 C
 -1.743 -0.247 -0.589
 -0.247 -1.136 1.656
 -0.589 1.656 0.708
 0.046 0.007 0.007
 0.007 0.030 -0.019
 0.007 -0.020 0.000

atensor 4 H
 4.721 0.122 -3.762
 0.122 0.275 -0.103
 -3.762 -0.103 4.112
 0.004 0.000 0.021
 0.000 0.015 0.001
 0.012 0.000 -0.003

atensor 5 C
-1.049 0.022 -1.757
0.022 -1.831 -0.048
-1.757 -0.048 0.707
0.027 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H
0.628 1.208 -1.065
1.208 4.369 -3.610
-1.065 -3.610 4.112
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.770 0.212 -0.497
0.212 -1.112 -1.686
-0.497 -1.686 0.707
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.301 -2.077 3.104
-2.077 1.695 -2.128
3.104 -2.128 4.112
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.299 -0.365 1.449
-0.365 -1.581 -0.994
1.449 -0.994 0.708
0.034 0.010 -0.017
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.069 2.152 2.983
2.152 1.927 2.295
2.983 2.295 4.113
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.340 0.378 1.393
0.378 -1.540 1.071
1.393 1.071 0.708
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.017 -0.013 0.000

atensor 12 H
0.627 1.208 1.065
1.208 4.368 3.610
1.065 3.610 4.112
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.769 0.212 0.497
0.212 -1.111 1.686

0.497 1.686 0.709
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.301 -2.076 -3.105
-2.076 1.695 2.128
-3.105 2.128 4.113
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.299 -0.365 -1.450
-0.365 -1.581 0.993
-1.450 0.993 0.709
0.034 0.010 0.017
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.069 2.152 -2.983
2.152 1.928 -2.295
-2.983 -2.295 4.112
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.340 0.378 -1.393
0.378 -1.540 -1.072
-1.393 -1.072 0.708
0.035 -0.010 0.016
-0.010 0.041 0.012
0.017 0.013 0.000

atensor 18 H
0.771 -1.406 1.261
-1.406 4.225 -3.546
1.261 -3.546 4.111
0.014 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.744 -0.247 0.589
-0.247 -1.136 -1.656
0.589 -1.656 0.707
0.046 0.007 -0.007
0.007 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.049 0.021 1.757
0.021 -1.831 0.048
1.757 0.048 0.708
0.027 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.721 0.122 3.762
0.122 0.274 0.103
3.762 0.103 4.111
0.004 0.000 -0.021
0.000 0.015 -0.001

-0.012 0.000 -0.003

orbtensor 1 V

-3088.084	-0.002	-0.019
-0.002	-3088.085	-0.146
-0.019	-0.146	-354.934
1709.344	0.000	0.000
0.000	1709.344	0.000
0.000	0.000	1715.988

orbtensor 2 H

-1.061	3.360	0.966
3.360	-9.316	-2.719
0.966	-2.719	-0.665
26.274	-4.309	-1.273
-4.309	36.860	3.581
-1.273	3.581	25.573

orbtensor 3 C

-155.939	23.789	10.753
23.789	-214.384	-30.260
10.753	-30.260	-59.550
226.307	-5.220	-4.702
-5.220	239.130	13.226
-4.702	13.226	222.717

orbtensor 4 H

-10.502	-0.292	2.884
-0.292	0.126	0.079
2.884	0.079	-0.665
38.381	0.375	-3.799
0.375	24.751	-0.104
-3.799	-0.104	25.572

orbtensor 5 C

-222.791	-2.067	32.095
-2.067	-147.533	0.878
32.095	0.878	-59.545
240.973	0.454	-14.032
0.454	224.459	-0.385
-14.032	-0.385	222.714

orbtensor 6 H

-0.717	-2.888	0.816
-2.888	-9.658	2.768
0.816	2.768	-0.664
25.833	3.703	-1.075
3.703	37.300	-3.646
-1.075	-3.646	25.572

orbtensor 7 C

-153.505	-20.448	9.077
-20.448	-216.819	30.797
9.077	30.797	-59.545
225.769	4.487	-3.970
4.487	239.663	-13.465
-3.970	-13.465	222.714

orbtensor 8 H

-7.107	4.964	-2.380
4.964	-3.269	1.632
-2.380	1.632	-0.665
34.028	-6.366	3.136
-6.366	29.105	-2.149
3.136	-2.149	25.572

orbtensor 9 C

-198.752	35.148	-26.493
35.148	-171.571	18.154
-26.493	18.154	-59.549
235.698	-7.712	11.580
-7.712	229.735	-7.937
11.580	-7.937	222.716

orbtensor 10 H

-6.553	-5.144	-2.287
-5.144	-3.824	-1.760
-2.287	-1.760	-0.665
33.317	6.597	3.013
6.597	29.817	2.318
3.013	2.318	25.573

orbtensor 11 C

-194.823	-36.421	-25.458
-36.421	-175.500	-19.586
-25.458	-19.586	-59.552
234.839	7.991	11.126
7.991	230.599	8.560
11.126	8.560	222.718

orbtensor 12 H

-0.718	-2.887	-0.816
-2.887	-9.659	-2.768
-0.816	-2.768	-0.665
25.834	3.703	1.075
3.703	37.300	3.646
1.075	3.646	25.573

orbtensor 13 C

-153.509	-20.445	-9.081
-20.445	-216.812	-30.813
-9.081	-30.813	-59.553
225.774	4.486	3.970
4.486	239.663	13.465
3.970	13.465	222.718

orbtensor 14 H

-7.108	4.963	2.380
4.963	-3.268	-1.632
2.380	-1.632	-0.665
34.029	-6.365	-3.136
-6.365	29.105	2.149
-3.136	2.149	25.573

orbtensor 15 C

-198.755	35.142	26.493
35.142	-171.568	-18.165
26.493	-18.165	-59.553
235.701	-7.710	-11.579
-7.710	229.735	7.937
-11.579	7.937	222.718

orbtensor 16 H

-6.553	-5.144	2.286
-5.144	-3.824	1.759
2.286	1.759	-0.665
33.317	6.597	-3.012
6.597	29.817	-2.317
-3.012	-2.317	25.572

orbtensor 17 C

-194.822	-36.426	25.450
-36.426	-175.505	19.570
25.450	19.570	-59.546

234.837 7.993 -11.125
 7.993 230.600 -8.559
 -11.125 -8.559 222.715

orbtensor 18 H
 -1.061 3.360 -0.966
 3.360 -9.316 2.718
 -0.966 2.718 -0.664
 26.273 -4.309 1.273
 -4.309 36.860 -3.580
 1.273 -3.580 25.572

orbtensor 19 C
 -155.936 23.791 -10.752
 23.791 -214.393 30.243
 -10.752 30.243 -59.542
 226.304 -5.220 4.702
 -5.220 239.132 -13.225
 4.702 -13.225 222.713

orbtensor 20 C
 -222.791 -2.063 -32.094
 -2.063 -147.536 -0.888
 -32.094 -0.888 -59.548
 240.975 0.452 14.031
 0.452 224.462 0.385
 14.031 0.385 222.715

orbtensor 21 H
 -10.503 -0.291 -2.884
 -0.291 0.125 -0.079
 -2.884 -0.079 -0.665
 38.382 0.374 3.799
 0.374 24.752 0.104
 3.799 0.104 25.572

gtensor (ppt)
 -0.126 0.000 0.000
 0.000 -0.126 0.000
 0.000 0.000 -0.132
 -6.413 0.000 0.000
 0.000 -6.413 0.000
 0.000 0.000 -1.286

zfstensor (cm-1)
 -0.757713 -0.000010 -0.000013
 -0.000010 -0.757663 -0.000088
 -0.000013 -0.000088 0.830610

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	1.9547	-465.47567	-981.06169	-39.39224	-1020.45393	-1485.92960
2	H	3.0417	25.88833	-402.05704	0.31188	-401.74516	-375.85682
3	C	-0.6983	86.09367	367.02509	1.63432	368.65941	454.75308
4	H	3.0413	25.88767	-402.01298	0.31210	-401.70088	-375.81321
5	C	-0.6993	86.09233	367.55066	1.63462	369.18527	455.27761
6	H	3.0417	25.88867	-402.05704	0.31219	-401.74485	-375.85618
7	C	-0.6997	86.09233	367.72585	1.63529	369.36114	455.45347
8	H	3.0413	25.88800	-402.01298	0.31218	-401.70080	-375.81280
9	C	-0.6987	86.09233	367.20028	1.63511	368.83538	454.92772
10	H	3.0417	25.88833	-402.05704	0.31216	-401.74488	-375.85655

11	C	-0.6987	86.09367	367.20028	1.63473	368.83501	454.92867
12	H	3.0410	25.88833	-401.96892	0.31205	-401.65687	-375.76853
13	C	-0.6983	86.09367	367.02509	1.63544	368.66053	454.75420
14	H	3.0417	25.88867	-402.05704	0.31222	-401.74482	-375.85615
15	C	-0.6983	86.09267	367.02509	1.63561	368.66069	454.75336
16	H	3.0417	25.88800	-402.05704	0.31211	-401.74493	-375.85693
17	C	-0.6987	86.09300	367.20028	1.63518	368.83546	454.92846
18	H	3.0413	25.88800	-402.01298	0.31199	-401.70099	-375.81299
19	C	-0.6990	86.09267	367.37547	1.63449	369.00996	455.10263
20	C	-0.6990	86.09233	367.37547	1.63528	369.01075	455.10308
21	H	3.0407	25.88767	-401.92486	0.31195	-401.61291	-375.72524
13C Average		-0.6988	86.09287	367.27035	1.63501	368.90536	454.99823
1H Average		3.0414	25.88817	-402.02179	0.31208	-401.70971	-375.82154

=====
4VCp2-STO-PBE-Pederson

Temperature: 298

Spin: 1.5

atensor 1 V

27.854 0.000 0.000
0.000 27.853 0.004
0.000 0.004 -28.684
-8.154 0.000 0.000
0.000 -8.154 0.000
0.000 0.000 -4.851

atensor 2 H

0.771 -1.406 -1.261
-1.406 4.225 3.546
-1.261 3.546 4.112
0.014 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

atensor 3 C

-1.743 -0.247 -0.589
-0.247 -1.136 1.656
-0.589 1.656 0.708
0.046 0.007 0.007
0.007 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H

4.721 0.122 -3.762
0.122 0.275 -0.103
-3.762 -0.103 4.112
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C

-1.049 0.022 -1.757
0.022 -1.831 -0.048
-1.757 -0.048 0.707
0.027 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H

0.628 1.208 -1.065
1.208 4.369 -3.610
-1.065 -3.610 4.112
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C
-1.770 0.212 -0.497
0.212 -1.112 -1.686
-0.497 -1.686 0.707
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H
3.301 -2.077 3.104
-2.077 1.695 -2.128
3.104 -2.128 4.112
0.008 0.005 -0.017
0.005 0.011 0.012
-0.010 0.007 -0.003

atensor 9 C
-1.299 -0.365 1.449
-0.365 -1.581 -0.994
1.449 -0.994 0.708
0.034 0.010 -0.017
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.069 2.152 2.983
2.152 1.927 2.295
2.983 2.295 4.113
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.340 0.378 1.393
0.378 -1.540 1.071
1.393 1.071 0.708
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.017 -0.013 0.000

atensor 12 H
0.627 1.208 1.065
1.208 4.368 3.610
1.065 3.610 4.112
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.769 0.212 0.497
0.212 -1.111 1.686
0.497 1.686 0.709
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.301 -2.076 -3.105
-2.076 1.695 2.128
-3.105 2.128 4.113
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.299 -0.365 -1.450

-0.365 -1.581 0.993
-1.450 0.993 0.709
0.034 0.010 0.017
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.069 2.152 -2.983
2.152 1.928 -2.295
-2.983 -2.295 4.112
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C
-1.340 0.378 -1.393
0.378 -1.540 -1.072
-1.393 -1.072 0.708
0.035 -0.010 0.016
-0.010 0.041 0.012
0.017 0.013 0.000

atensor 18 H
0.771 -1.406 1.261
-1.406 4.225 -3.546
1.261 -3.546 4.111
0.014 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.744 -0.247 0.589
-0.247 -1.136 -1.656
0.589 -1.656 0.707
0.046 0.007 -0.007
0.007 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.049 0.021 1.757
0.021 -1.831 0.048
1.757 0.048 0.708
0.027 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.721 0.122 3.762
0.122 0.274 0.103
3.762 0.103 4.111
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3088.084 -0.002 -0.019
-0.002 -3088.085 -0.146
-0.019 -0.146 -354.934
1709.344 0.000 0.000
0.000 1709.344 0.000
0.000 0.000 1715.988

orbtensor 2 H
-1.061 3.360 0.966
3.360 -9.316 -2.719
0.966 -2.719 -0.665
26.274 -4.309 -1.273

-4.309 36.860 3.581
-1.273 3.581 25.573

orbtensor 3 C
-155.939 23.789 10.753
23.789 -214.384 -30.260
10.753 -30.260 -59.550
226.307 -5.220 -4.702
-5.220 239.130 13.226
-4.702 13.226 222.717

orbtensor 4 H
-10.502 -0.292 2.884
-0.292 0.126 0.079
2.884 0.079 -0.665
38.381 0.375 -3.799
0.375 24.751 -0.104
-3.799 -0.104 25.572

orbtensor 5 C
-222.791 -2.067 32.095
-2.067 -147.533 0.878
32.095 0.878 -59.545
240.973 0.454 -14.032
0.454 224.459 -0.385
-14.032 -0.385 222.714

orbtensor 6 H
-0.717 -2.888 0.816
-2.888 -9.658 2.768
0.816 2.768 -0.664
25.833 3.703 -1.075
3.703 37.300 -3.646
-1.075 -3.646 25.572

orbtensor 7 C
-153.505 -20.448 9.077
-20.448 -216.819 30.797
9.077 30.797 -59.545
225.769 4.487 -3.970
4.487 239.663 -13.465
-3.970 -13.465 222.714

orbtensor 8 H
-7.107 4.964 -2.380
4.964 -3.269 1.632
-2.380 1.632 -0.665
34.028 -6.366 3.136
-6.366 29.105 -2.149
3.136 -2.149 25.572

orbtensor 9 C
-198.752 35.148 -26.493
35.148 -171.571 18.154
-26.493 18.154 -59.549
235.698 -7.712 11.580
-7.712 229.735 -7.937
11.580 -7.937 222.716

orbtensor 10 H
-6.553 -5.144 -2.287
-5.144 -3.824 -1.760
-2.287 -1.760 -0.665
33.317 6.597 3.013
6.597 29.817 2.318
3.013 2.318 25.573

orbtensor 11 C
-194.823 -36.421 -25.458
-36.421 -175.500 -19.586
-25.458 -19.586 -59.552
234.839 7.991 11.126
7.991 230.599 8.560
11.126 8.560 222.718

orbtensor 12 H
-0.718 -2.887 -0.816
-2.887 -9.659 -2.768
-0.816 -2.768 -0.665
25.834 3.703 1.075
3.703 37.300 3.646
1.075 3.646 25.573

orbtensor 13 C
-153.509 -20.445 -9.081
-20.445 -216.812 -30.813
-9.081 -30.813 -59.553
225.774 4.486 3.970
4.486 239.663 13.465
3.970 13.465 222.718

orbtensor 14 H
-7.108 4.963 2.380
4.963 -3.268 -1.632
2.380 -1.632 -0.665
34.029 -6.365 -3.136
-6.365 29.105 2.149
-3.136 2.149 25.573

orbtensor 15 C
-198.755 35.142 26.493
35.142 -171.568 -18.165
26.493 -18.165 -59.553
235.701 -7.710 -11.579
-7.710 229.735 7.937
-11.579 7.937 222.718

orbtensor 16 H
-6.553 -5.144 2.286
-5.144 -3.824 1.759
2.286 1.759 -0.665
33.317 6.597 -3.012
6.597 29.817 -2.317
-3.012 -2.317 25.572

orbtensor 17 C
-194.822 -36.426 25.450
-36.426 -175.505 19.570
25.450 19.570 -59.546
234.837 7.993 -11.125
7.993 230.600 -8.559
-11.125 -8.559 222.715

orbtensor 18 H
-1.061 3.360 -0.966
3.360 -9.316 2.718
-0.966 2.718 -0.664
26.273 -4.309 1.273
-4.309 36.860 -3.580
1.273 -3.580 25.572

orbtensor 19 C
-155.936 23.791 -10.752
23.791 -214.393 30.243

```

-10.752  30.243  -59.542
226.304  -5.220   4.702
-5.220  239.132  -13.225
4.702   -13.225  222.713

```

```

orbtensor 20 C
-222.791  -2.063  -32.094
-2.063  -147.536  -0.888
-32.094  -0.888  -59.548
240.975   0.452  14.031
0.452   224.462   0.385
14.031   0.385  222.715

```

```

orbtensor 21 H
-10.503  -0.291  -2.884
-0.291   0.125  -0.079
-2.884  -0.079  -0.665
38.382   0.374   3.799
0.374   24.752   0.104
3.799   0.104  25.572

```

```

gtensor (ppt)
-0.126   0.000   0.000
0.000  -0.126   0.000
0.000   0.000  -0.132
-6.413   0.000   0.000
0.000  -6.413   0.000
0.000   0.000  -1.286

```

```

zfstensor (cm-1)
-0.300410  0.000000  -0.000005
 0.000000  -0.300410   0.000049
-0.000005  0.000049   0.600821

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	1.9547	-465.47567	-981.06912	-15.78458	-996.85370	-1462.32937
2	H	3.0417	25.88833	-402.06009	0.12511	-401.93497	-376.04664
3	C	-0.6983	86.09367	367.02787	0.65515	367.68302	453.77668
4	H	3.0413	25.88767	-402.01603	0.12507	-401.89096	-376.00329
5	C	-0.6993	86.09233	367.55345	0.65499	368.20844	454.30077
6	H	3.0417	25.88867	-402.06009	0.12493	-401.93515	-376.04649
7	C	-0.6997	86.09233	367.72864	0.65498	368.38361	454.47595
8	H	3.0413	25.88800	-402.01603	0.12500	-401.89103	-376.00303
9	C	-0.6987	86.09233	367.20306	0.65502	367.85808	453.95042
10	H	3.0417	25.88833	-402.06009	0.12519	-401.93490	-376.04657
11	C	-0.6987	86.09367	367.20306	0.65523	367.85829	453.95195
12	H	3.0410	25.88833	-401.97196	0.12519	-401.84678	-375.95844
13	C	-0.6983	86.09367	367.02787	0.65561	367.68348	453.77714
14	H	3.0417	25.88867	-402.06009	0.12520	-401.93489	-376.04622
15	C	-0.6983	86.09267	367.02787	0.65556	367.68343	453.77609
16	H	3.0417	25.88800	-402.06009	0.12497	-401.93512	-376.04712
17	C	-0.6987	86.09300	367.20306	0.65504	367.85811	453.95111
18	H	3.0413	25.88800	-402.01603	0.12485	-401.89117	-376.00317
19	C	-0.6990	86.09267	367.37825	0.65466	368.03291	454.12558
20	C	-0.6990	86.09233	367.37825	0.65528	368.03353	454.12586
21	H	3.0407	25.88767	-401.92790	0.12501	-401.80289	-375.91522
13C Average		-0.6988	86.09287	367.27314	0.65515	367.92829	454.02116
1H Average		3.0414	25.88817	-402.02484	0.12505	-401.89979	-376.01162

=====
4VCp2-STO-PBE-Van-Wullen

Temperature: 298

Spin: 1.5

atensor 1 V

27.854 0.000 0.000
0.000 27.853 0.004
0.000 0.004 -28.684
-8.154 0.000 0.000
0.000 -8.154 0.000
0.000 0.000 -4.851

atensor 2 H

0.771 -1.406 -1.261
-1.406 4.225 3.546
-1.261 3.546 4.112
0.014 0.003 0.007
0.003 0.006 -0.020
0.004 -0.011 -0.003

atensor 3 C

-1.743 -0.247 -0.589
-0.247 -1.136 1.656
-0.589 1.656 0.708
0.046 0.007 0.007
0.007 0.030 -0.019
0.007 -0.020 0.000

atensor 4 H

4.721 0.122 -3.762
0.122 0.275 -0.103
-3.762 -0.103 4.112
0.004 0.000 0.021
0.000 0.015 0.001
0.012 0.000 -0.003

atensor 5 C

-1.049 0.022 -1.757
0.022 -1.831 -0.048
-1.757 -0.048 0.707
0.027 -0.001 0.020
-0.001 0.048 0.001
0.021 0.001 0.000

atensor 6 H

0.628 1.208 -1.065
1.208 4.369 -3.610
-1.065 -3.610 4.112
0.014 -0.003 0.006
-0.003 0.005 0.020
0.003 0.011 -0.003

atensor 7 C

-1.770 0.212 -0.497
0.212 -1.112 -1.686
-0.497 -1.686 0.707
0.047 -0.006 0.006
-0.006 0.029 0.019
0.006 0.020 0.000

atensor 8 H

3.301 -2.077 3.104
-2.077 1.695 -2.128
3.104 -2.128 4.112
0.008 0.005 -0.017
0.005 0.011 0.012

-0.010 0.007 -0.003

atensor 9 C
-1.299 -0.365 1.449
-0.365 -1.581 -0.994
1.449 -0.994 0.708
0.034 0.010 -0.017
0.010 0.042 0.011
-0.017 0.012 0.000

atensor 10 H
3.069 2.152 2.983
2.152 1.927 2.295
2.983 2.295 4.113
0.008 -0.005 -0.017
-0.005 0.011 -0.013
-0.009 -0.007 -0.003

atensor 11 C
-1.340 0.378 1.393
0.378 -1.540 1.071
1.393 1.071 0.708
0.035 -0.010 -0.016
-0.010 0.041 -0.012
-0.017 -0.013 0.000

atensor 12 H
0.627 1.208 1.065
1.208 4.368 3.610
1.065 3.610 4.112
0.014 -0.003 -0.006
-0.003 0.005 -0.020
-0.003 -0.011 -0.003

atensor 13 C
-1.769 0.212 0.497
0.212 -1.111 1.686
0.497 1.686 0.709
0.047 -0.006 -0.006
-0.006 0.029 -0.019
-0.006 -0.020 0.000

atensor 14 H
3.301 -2.076 -3.105
-2.076 1.695 2.128
-3.105 2.128 4.113
0.008 0.005 0.017
0.005 0.011 -0.012
0.010 -0.007 -0.003

atensor 15 C
-1.299 -0.365 -1.450
-0.365 -1.581 0.993
-1.450 0.993 0.709
0.034 0.010 0.017
0.010 0.042 -0.011
0.017 -0.012 0.000

atensor 16 H
3.069 2.152 -2.983
2.152 1.928 -2.295
-2.983 -2.295 4.112
0.008 -0.005 0.017
-0.005 0.011 0.013
0.009 0.007 -0.003

atensor 17 C

-1.340 0.378 -1.393
0.378 -1.540 -1.072
-1.393 -1.072 0.708
0.035 -0.010 0.016
-0.010 0.041 0.012
0.017 0.013 0.000

atensor 18 H
0.771 -1.406 1.261
-1.406 4.225 -3.546
1.261 -3.546 4.111
0.014 0.003 -0.007
0.003 0.006 0.020
-0.004 0.011 -0.003

atensor 19 C
-1.744 -0.247 0.589
-0.247 -1.136 -1.656
0.589 -1.656 0.707
0.046 0.007 -0.007
0.007 0.030 0.019
-0.007 0.020 0.000

atensor 20 C
-1.049 0.021 1.757
0.021 -1.831 0.048
1.757 0.048 0.708
0.027 -0.001 -0.020
-0.001 0.048 -0.001
-0.021 -0.001 0.000

atensor 21 H
4.721 0.122 3.762
0.122 0.274 0.103
3.762 0.103 4.111
0.004 0.000 -0.021
0.000 0.015 -0.001
-0.012 0.000 -0.003

orbtensor 1 V
-3088.084 -0.002 -0.019
-0.002 -3088.085 -0.146
-0.019 -0.146 -354.934
1709.344 0.000 0.000
0.000 1709.344 0.000
0.000 0.000 1715.988

orbtensor 2 H
-1.061 3.360 0.966
3.360 -9.316 -2.719
0.966 -2.719 -0.665
26.274 -4.309 -1.273
-4.309 36.860 3.581
-1.273 3.581 25.573

orbtensor 3 C
-155.939 23.789 10.753
23.789 -214.384 -30.260
10.753 -30.260 -59.550
226.307 -5.220 -4.702
-5.220 239.130 13.226
-4.702 13.226 222.717

orbtensor 4 H
-10.502 -0.292 2.884
-0.292 0.126 0.079
2.884 0.079 -0.665

38.381	0.375	-3.799
0.375	24.751	-0.104
-3.799	-0.104	25.572

orbtensor 5 C

-222.791	-2.067	32.095
-2.067	-147.533	0.878
32.095	0.878	-59.545
240.973	0.454	-14.032
0.454	224.459	-0.385
-14.032	-0.385	222.714

orbtensor 6 H

-0.717	-2.888	0.816
-2.888	-9.658	2.768
0.816	2.768	-0.664
25.833	3.703	-1.075
3.703	37.300	-3.646
-1.075	-3.646	25.572

orbtensor 7 C

-153.505	-20.448	9.077
-20.448	-216.819	30.797
9.077	30.797	-59.545
225.769	4.487	-3.970
4.487	239.663	-13.465
-3.970	-13.465	222.714

orbtensor 8 H

-7.107	4.964	-2.380
4.964	-3.269	1.632
-2.380	1.632	-0.665
34.028	-6.366	3.136
-6.366	29.105	-2.149
3.136	-2.149	25.572

orbtensor 9 C

-198.752	35.148	-26.493
35.148	-171.571	18.154
-26.493	18.154	-59.549
235.698	-7.712	11.580
-7.712	229.735	-7.937
11.580	-7.937	222.716

orbtensor 10 H

-6.553	-5.144	-2.287
-5.144	-3.824	-1.760
-2.287	-1.760	-0.665
33.317	6.597	3.013
6.597	29.817	2.318
3.013	2.318	25.573

orbtensor 11 C

-194.823	-36.421	-25.458
-36.421	-175.500	-19.586
-25.458	-19.586	-59.552
234.839	7.991	11.126
7.991	230.599	8.560
11.126	8.560	222.718

orbtensor 12 H

-0.718	-2.887	-0.816
-2.887	-9.659	-2.768
-0.816	-2.768	-0.665
25.834	3.703	1.075
3.703	37.300	3.646
1.075	3.646	25.573

orbtensor 13 C
-153.509 -20.445 -9.081
-20.445 -216.812 -30.813
-9.081 -30.813 -59.553
225.774 4.486 3.970
4.486 239.663 13.465
3.970 13.465 222.718

orbtensor 14 H
-7.108 4.963 2.380
4.963 -3.268 -1.632
2.380 -1.632 -0.665
34.029 -6.365 -3.136
-6.365 29.105 2.149
-3.136 2.149 25.573

orbtensor 15 C
-198.755 35.142 26.493
35.142 -171.568 -18.165
26.493 -18.165 -59.553
235.701 -7.710 -11.579
-7.710 229.735 7.937
-11.579 7.937 222.718

orbtensor 16 H
-6.553 -5.144 2.286
-5.144 -3.824 1.759
2.286 1.759 -0.665
33.317 6.597 -3.012
6.597 29.817 -2.317
-3.012 -2.317 25.572

orbtensor 17 C
-194.822 -36.426 25.450
-36.426 -175.505 19.570
25.450 19.570 -59.546
234.837 7.993 -11.125
7.993 230.600 -8.559
-11.125 -8.559 222.715

orbtensor 18 H
-1.061 3.360 -0.966
3.360 -9.316 2.718
-0.966 2.718 -0.664
26.273 -4.309 1.273
-4.309 36.860 -3.580
1.273 -3.580 25.572

orbtensor 19 C
-155.936 23.791 -10.752
23.791 -214.393 30.243
-10.752 30.243 -59.542
226.304 -5.220 4.702
-5.220 239.132 -13.225
4.702 -13.225 222.713

orbtensor 20 C
-222.791 -2.063 -32.094
-2.063 -147.536 -0.888
-32.094 -0.888 -59.548
240.975 0.452 14.031
0.452 224.462 0.385
14.031 0.385 222.715

orbtensor 21 H
-10.503 -0.291 -2.884

```

-0.291    0.125   -0.079
-2.884   -0.079   -0.665
38.382    0.374    3.799
0.374    24.752    0.104
3.799     0.104    25.572

```

```

gtensor (ppt)
-0.126    0.000    0.000
0.000   -0.126    0.000
0.000    0.000   -0.132
-6.413    0.000    0.000
0.000   -6.413    0.000
0.000    0.000   -1.286

```

```

zfstensor (cm-1)
-0.450615  0.000000  -0.000007
 0.000000  -0.450615  0.000073
-0.000007  0.000073  0.901231

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	1.9547	-465.47567	-981.06457	-31.27079	-1012.33536	-1477.81103
2	H	3.0417	25.88833	-402.05822	0.24782	-401.81041	-375.92207
3	C	-0.6983	86.09367	367.02617	1.29783	368.32400	454.41766
4	H	3.0413	25.88767	-402.01416	0.24777	-401.76639	-375.87873
5	C	-0.6993	86.09233	367.55174	1.29760	368.84934	454.94167
6	H	3.0417	25.88867	-402.05822	0.24755	-401.81067	-375.92201
7	C	-0.6997	86.09233	367.72693	1.29765	369.02458	455.11691
8	H	3.0413	25.88800	-402.01416	0.24767	-401.76649	-375.87849
9	C	-0.6987	86.09233	367.20136	1.29772	368.49908	454.59141
10	H	3.0417	25.88833	-402.05822	0.24799	-401.81024	-375.92190
11	C	-0.6987	86.09367	367.20136	1.29803	368.49938	454.59305
12	H	3.0410	25.88833	-401.97010	0.24796	-401.72213	-375.83380
13	C	-0.6983	86.09367	367.02617	1.29874	368.32491	454.41858
14	H	3.0417	25.88867	-402.05822	0.24800	-401.81022	-375.92155
15	C	-0.6983	86.09267	367.02617	1.29867	368.32483	454.41750
16	H	3.0417	25.88800	-402.05822	0.24760	-401.81062	-375.92262
17	C	-0.6987	86.09300	367.20136	1.29775	368.49911	454.59211
18	H	3.0413	25.88800	-402.01416	0.24739	-401.76677	-375.87877
19	C	-0.6990	86.09267	367.37655	1.29702	368.67357	454.76624
20	C	-0.6990	86.09233	367.37655	1.29818	368.67473	454.76706
21	H	3.0407	25.88767	-401.92604	0.24767	-401.67837	-375.79070
13C Average		-0.6988	86.09287	367.27143	1.29792	368.56935	454.66222
1H Average		3.0414	25.88817	-402.02297	0.24774	-401.77523	-375.88706

```

=====
4VcP2-STO-PBE0-No-ZFS
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
-22.285 0.000 0.000
0.000 -22.286 0.003
0.000 0.003 -79.619
-10.115 0.000 0.000
0.000 -10.115 0.000
0.000 0.000 -4.441

```

```

atensor 2 H
0.630 -1.369 -1.301

```

-1.369 3.994 3.658
-1.301 3.658 3.896
0.019 0.007 0.011
0.007 0.002 -0.031
0.004 -0.010 -0.002

atensor 3 C
-1.923 -0.259 -0.597
-0.259 -1.286 1.678
-0.597 1.678 0.072
0.051 0.007 0.009
0.007 0.033 -0.026
0.007 -0.020 0.001

atensor 4 H
4.478 0.119 -3.881
0.119 0.146 -0.107
-3.881 -0.107 3.895
0.000 -0.001 0.032
-0.001 0.022 0.001
0.011 0.000 -0.002

atensor 5 C
-1.194 0.023 -1.780
0.023 -2.015 -0.049
-1.780 -0.049 0.071
0.031 -0.001 0.028
-0.001 0.053 0.001
0.021 0.001 0.001

atensor 6 H
0.490 1.177 -1.098
1.177 4.134 -3.724
-1.098 -3.724 3.896
0.020 -0.006 0.009
-0.006 0.001 0.031
0.003 0.010 -0.002

atensor 7 C
-1.950 0.223 -0.504
0.223 -1.260 -1.708
-0.504 -1.708 0.071
0.052 -0.006 0.008
-0.006 0.033 0.027
0.006 0.020 0.001

atensor 8 H
3.094 -2.023 3.203
-2.023 1.530 -2.195
3.202 -2.195 3.896
0.007 0.010 -0.027
0.010 0.015 0.018
-0.009 0.006 -0.002

atensor 9 C
-1.457 -0.383 1.469
-0.383 -1.753 -1.007
1.469 -1.007 0.072
0.038 0.011 -0.023
0.011 0.046 0.016
-0.017 0.012 0.001

atensor 10 H
2.868 2.096 3.078
2.096 1.756 2.368
3.077 2.368 3.897
0.008 -0.011 -0.026

-0.011 0.014 -0.020
-0.008 -0.007 -0.002

atensor 11 C
-1.499 0.397 1.412
0.397 -1.710 1.086
1.412 1.086 0.073
0.039 -0.011 -0.022
-0.011 0.045 -0.017
-0.016 -0.013 0.001

atensor 12 H
0.490 1.177 1.098
1.177 4.133 3.724
1.098 3.724 3.896
0.020 -0.006 -0.009
-0.006 0.001 -0.031
-0.003 -0.010 -0.002

atensor 13 C
-1.949 0.223 0.504
0.223 -1.259 1.708
0.504 1.708 0.073
0.052 -0.006 -0.008
-0.006 0.033 -0.027
-0.006 -0.020 0.001

atensor 14 H
3.094 -2.022 -3.203
-2.022 1.529 2.195
-3.203 2.195 3.897
0.007 0.010 0.027
0.010 0.015 -0.018
0.009 -0.006 -0.002

atensor 15 C
-1.456 -0.383 -1.469
-0.383 -1.753 1.007
-1.469 1.007 0.073
0.038 0.011 0.023
0.011 0.046 -0.016
0.017 -0.012 0.001

atensor 16 H
2.868 2.096 -3.077
2.096 1.756 -2.368
-3.077 -2.368 3.896
0.008 -0.011 0.026
-0.011 0.014 0.020
0.008 0.007 -0.002

atensor 17 C
-1.499 0.397 -1.411
0.397 -1.710 -1.086
-1.411 -1.086 0.072
0.039 -0.011 0.022
-0.011 0.045 0.017
0.016 0.013 0.001

atensor 18 H
0.630 -1.369 1.301
-1.369 3.994 -3.659
1.301 -3.658 3.895
0.019 0.007 -0.011
0.007 0.002 0.031
-0.004 0.010 -0.002

atensor 19 C
-1.923 -0.260 0.597
-0.260 -1.286 -1.678
0.597 -1.678 0.071
0.051 0.007 -0.009
0.007 0.033 0.026
-0.007 0.020 0.001

atensor 20 C
-1.194 0.022 1.780
0.022 -2.015 0.049
1.780 0.049 0.072
0.031 -0.001 -0.028
-0.001 0.053 -0.001
-0.021 -0.001 0.001

atensor 21 H
4.477 0.119 3.881
0.119 0.146 0.106
3.881 0.106 3.895
0.000 -0.001 -0.032
-0.001 0.022 -0.001
-0.011 0.000 -0.002

orbtensor 1 V
-3623.426 0.000 -0.022
0.000 -3623.422 -0.191
-0.022 -0.191 -252.559
1698.012 0.000 0.000
0.000 1698.012 -0.001
0.000 -0.001 1714.727

orbtensor 2 H
-1.361 4.360 0.780
4.360 -12.074 -2.194
0.780 -2.194 -0.316
27.507 -5.032 -0.945
-5.032 39.872 2.658
-0.945 2.658 25.134

orbtensor 3 C
-183.081 16.919 7.766
16.919 -224.649 -21.861
7.766 -21.861 -67.067
255.247 2.404 -1.469
2.404 249.338 4.133
-1.469 4.133 233.537

orbtensor 4 H
-13.614 -0.379 2.327
-0.379 0.180 0.064
2.327 0.064 -0.316
41.649 0.437 -2.820
0.437 25.729 -0.077
-2.820 -0.077 25.134

orbtensor 5 C
-230.630 -1.469 23.181
-1.469 -177.106 0.632
23.181 0.632 -67.065
248.490 -0.208 -4.385
-0.208 256.094 -0.119
-4.385 -0.119 233.537

orbtensor 6 H
-0.914 -3.748 0.659
-3.748 -12.519 2.234

0.659	2.234	-0.315
26.991	4.325	-0.798
4.325	40.386	-2.706
-0.798	-2.706	25.133

orbtensor 7 C

-181.352	-14.543	6.555
-14.543	-226.382	22.244
6.555	22.244	-67.065
255.490	-2.065	-1.240
-2.065	249.094	-4.207
-1.240	-4.207	233.537

orbtensor 8 H

-9.207	6.443	-1.922
6.443	-4.224	1.317
-1.922	1.317	-0.315
36.564	-7.437	2.328
-7.437	30.812	-1.596
2.328	-1.596	25.133

orbtensor 9 C

-213.530	24.998	-19.139
24.998	-194.198	13.112
-19.139	13.112	-67.068
250.918	3.551	3.620
3.551	253.665	-2.480
3.620	-2.480	233.538

orbtensor 10 H

-8.488	-6.676	-1.846
-6.676	-4.945	-1.421
-1.846	-1.421	-0.316
35.733	7.706	2.237
7.706	31.644	1.721
2.237	1.721	25.134

orbtensor 11 C

-210.734	-25.904	-18.392
-25.904	-196.992	-14.150
-18.392	-14.150	-67.069
251.315	-3.681	3.477
-3.681	253.268	2.676
3.477	2.676	233.538

orbtensor 12 H

-0.914	-3.748	-0.659
-3.748	-12.519	-2.235
-0.659	-2.235	-0.316
26.991	4.325	0.798
4.325	40.386	2.708
0.798	2.708	25.134

orbtensor 13 C

-181.352	-14.541	-6.559
-14.541	-226.374	-22.261
-6.559	-22.261	-67.071
255.491	-2.066	1.240
-2.066	249.093	4.209
1.240	4.209	233.539

orbtensor 14 H

-9.208	6.443	1.922
6.443	-4.224	-1.317
1.922	-1.317	-0.316
36.564	-7.436	-2.329
-7.436	30.812	1.596

```

-2.329    1.596    25.133

orbtensor 15 C
-213.532   24.994   19.138
24.994  -194.195  -13.125
19.138   -13.125  -67.071
250.918    3.551   -3.619
3.551   253.664    2.482
-3.619    2.482   233.538

orbtensor 16 H
-8.488   -6.677    1.845
-6.677   -4.946    1.420
1.845    1.420   -0.316
35.733    7.706   -2.236
7.706   31.645   -1.720
-2.236   -1.720   25.133

orbtensor 17 C
-210.735  -25.907   18.385
-25.907  -196.997   14.133
18.385   14.133  -67.065
251.316   -3.680   -3.477
-3.680   253.269   -2.674
-3.477   -2.674   233.537

orbtensor 18 H
-1.360    4.360   -0.780
4.360  -12.074    2.193
-0.780    2.193   -0.316
27.506   -5.033    0.945
-5.033   39.872   -2.657
0.945   -2.657   25.133

orbtensor 19 C
-183.081   16.920   -7.766
16.920  -224.655   21.842
-7.766   21.842  -67.062
255.246    2.404    1.470
2.404   249.339   -4.132
1.470   -4.132   233.536

orbtensor 20 C
-230.628   -1.467  -23.182
-1.467  -177.106   -0.645
-23.182   -0.645  -67.066
248.490   -0.209    4.384
-0.209   256.095    0.122
4.384    0.122   233.537

orbtensor 21 H
-13.614   -0.379   -2.327
-0.379    0.179   -0.064
-2.327   -0.064   -0.316
41.649    0.437    2.820
0.437   25.729    0.077
2.820    0.077   25.134

gtensor (ppt)
-0.146    0.000    0.000
0.000   -0.146    0.000
0.000    0.000   -0.130
-11.659    0.000    0.000
0.000  -11.659   -0.001
0.000   -0.001   -0.935

```

averaging

13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-49.6203	-796.21867	24862.83404	30.98042	24893.81445	24097.59579
2	H	2.8463	26.25400	-375.60309	-0.24804	-375.85113	-349.59713
3	C	-1.0173	87.77500	533.78160	-1.02677	532.75482	620.52982
4	H	2.8463	26.25400	-375.60309	-0.24797	-375.85106	-349.59706
5	C	-1.0177	87.77333	533.95649	-1.02644	532.93005	620.70338
6	H	2.8463	26.25400	-375.60309	-0.24836	-375.85145	-349.59745
7	C	-1.0177	87.77400	533.95649	-1.02673	532.92976	620.70376
8	H	2.8467	26.25433	-375.64708	-0.24822	-375.89529	-349.64096
9	C	-1.0177	87.77500	533.95649	-1.02755	532.92894	620.70394
10	H	2.8470	26.25400	-375.69106	-0.24818	-375.93924	-349.68524
11	C	-1.0170	87.77533	533.60670	-1.02750	532.57920	620.35453
12	H	2.8460	26.25400	-375.55910	-0.24812	-375.80722	-349.55322
13	C	-1.0163	87.77533	533.25691	-1.02677	532.23014	620.00548
14	H	2.8467	26.25367	-375.64708	-0.24826	-375.89534	-349.64167
15	C	-1.0170	87.77400	533.60670	-1.02752	532.57918	620.35318
16	H	2.8467	26.25367	-375.64708	-0.24823	-375.89530	-349.64163
17	C	-1.0173	87.77500	533.78160	-1.02725	532.75435	620.52935
18	H	2.8460	26.25367	-375.55910	-0.24820	-375.80731	-349.55364
19	C	-1.0177	87.77433	533.95649	-1.02672	532.92977	620.70410
20	C	-1.0173	87.77400	533.78160	-1.02705	532.75454	620.52854
21	H	2.8460	26.25367	-375.55910	-0.24804	-375.80714	-349.55347
13C Average		-1.0173	87.77453	533.76411	-1.02703	532.73708	620.51161
1H Average		2.8464	26.25390	-375.61189	-0.24816	-375.86005	-349.60615

4VCp2-STO-PBE0-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 V
 -22.285 0.000 0.000
 0.000 -22.286 0.003
 0.000 0.003 -79.619
 -10.115 0.000 0.000
 0.000 -10.115 0.000
 0.000 0.000 -4.441

atensor 2 H
 0.630 -1.369 -1.301
 -1.369 3.994 3.658
 -1.301 3.658 3.896
 0.019 0.007 0.011
 0.007 0.002 -0.031
 0.004 -0.010 -0.002

atensor 3 C
 -1.923 -0.259 -0.597
 -0.259 -1.286 1.678
 -0.597 1.678 0.072
 0.051 0.007 0.009
 0.007 0.033 -0.026
 0.007 -0.020 0.001

atensor 4 H
 4.478 0.119 -3.881
 0.119 0.146 -0.107
 -3.881 -0.107 3.895
 0.000 -0.001 0.032
 -0.001 0.022 0.001

0.011 0.000 -0.002

atensor 5 C
-1.194 0.023 -1.780
0.023 -2.015 -0.049
-1.780 -0.049 0.071
0.031 -0.001 0.028
-0.001 0.053 0.001
0.021 0.001 0.001

atensor 6 H
0.490 1.177 -1.098
1.177 4.134 -3.724
-1.098 -3.724 3.896
0.020 -0.006 0.009
-0.006 0.001 0.031
0.003 0.010 -0.002

atensor 7 C
-1.950 0.223 -0.504
0.223 -1.260 -1.708
-0.504 -1.708 0.071
0.052 -0.006 0.008
-0.006 0.033 0.027
0.006 0.020 0.001

atensor 8 H
3.094 -2.023 3.203
-2.023 1.530 -2.195
3.202 -2.195 3.896
0.007 0.010 -0.027
0.010 0.015 0.018
-0.009 0.006 -0.002

atensor 9 C
-1.457 -0.383 1.469
-0.383 -1.753 -1.007
1.469 -1.007 0.072
0.038 0.011 -0.023
0.011 0.046 0.016
-0.017 0.012 0.001

atensor 10 H
2.868 2.096 3.078
2.096 1.756 2.368
3.077 2.368 3.897
0.008 -0.011 -0.026
-0.011 0.014 -0.020
-0.008 -0.007 -0.002

atensor 11 C
-1.499 0.397 1.412
0.397 -1.710 1.086
1.412 1.086 0.073
0.039 -0.011 -0.022
-0.011 0.045 -0.017
-0.016 -0.013 0.001

atensor 12 H
0.490 1.177 1.098
1.177 4.133 3.724
1.098 3.724 3.896
0.020 -0.006 -0.009
-0.006 0.001 -0.031
-0.003 -0.010 -0.002

atensor 13 C

-1.949 0.223 0.504
0.223 -1.259 1.708
0.504 1.708 0.073
0.052 -0.006 -0.008
-0.006 0.033 -0.027
-0.006 -0.020 0.001

atensor 14 H
3.094 -2.022 -3.203
-2.022 1.529 2.195
-3.203 2.195 3.897
0.007 0.010 0.027
0.010 0.015 -0.018
0.009 -0.006 -0.002

atensor 15 C
-1.456 -0.383 -1.469
-0.383 -1.753 1.007
-1.469 1.007 0.073
0.038 0.011 0.023
0.011 0.046 -0.016
0.017 -0.012 0.001

atensor 16 H
2.868 2.096 -3.077
2.096 1.756 -2.368
-3.077 -2.368 3.896
0.008 -0.011 0.026
-0.011 0.014 0.020
0.008 0.007 -0.002

atensor 17 C
-1.499 0.397 -1.411
0.397 -1.710 -1.086
-1.411 -1.086 0.072
0.039 -0.011 0.022
-0.011 0.045 0.017
0.016 0.013 0.001

atensor 18 H
0.630 -1.369 1.301
-1.369 3.994 -3.659
1.301 -3.658 3.895
0.019 0.007 -0.011
0.007 0.002 0.031
-0.004 0.010 -0.002

atensor 19 C
-1.923 -0.260 0.597
-0.260 -1.286 -1.678
0.597 -1.678 0.071
0.051 0.007 -0.009
0.007 0.033 0.026
-0.007 0.020 0.001

atensor 20 C
-1.194 0.022 1.780
0.022 -2.015 0.049
1.780 0.049 0.072
0.031 -0.001 -0.028
-0.001 0.053 -0.001
-0.021 -0.001 0.001

atensor 21 H
4.477 0.119 3.881
0.119 0.146 0.106
3.881 0.106 3.895

0.000 -0.001 -0.032
-0.001 0.022 -0.001
-0.011 0.000 -0.002

orbtensor 1 V
-3623.426 0.000 -0.022
0.000 -3623.422 -0.191
-0.022 -0.191 -252.559
1698.012 0.000 0.000
0.000 1698.012 -0.001
0.000 -0.001 1714.727

orbtensor 2 H
-1.361 4.360 0.780
4.360 -12.074 -2.194
0.780 -2.194 -0.316
27.507 -5.032 -0.945
-5.032 39.872 2.658
-0.945 2.658 25.134

orbtensor 3 C
-183.081 16.919 7.766
16.919 -224.649 -21.861
7.766 -21.861 -67.067
255.247 2.404 -1.469
2.404 249.338 4.133
-1.469 4.133 233.537

orbtensor 4 H
-13.614 -0.379 2.327
-0.379 0.180 0.064
2.327 0.064 -0.316
41.649 0.437 -2.820
0.437 25.729 -0.077
-2.820 -0.077 25.134

orbtensor 5 C
-230.630 -1.469 23.181
-1.469 -177.106 0.632
23.181 0.632 -67.065
248.490 -0.208 -4.385
-0.208 256.094 -0.119
-4.385 -0.119 233.537

orbtensor 6 H
-0.914 -3.748 0.659
-3.748 -12.519 2.234
0.659 2.234 -0.315
26.991 4.325 -0.798
4.325 40.386 -2.706
-0.798 -2.706 25.133

orbtensor 7 C
-181.352 -14.543 6.555
-14.543 -226.382 22.244
6.555 22.244 -67.065
255.490 -2.065 -1.240
-2.065 249.094 -4.207
-1.240 -4.207 233.537

orbtensor 8 H
-9.207 6.443 -1.922
6.443 -4.224 1.317
-1.922 1.317 -0.315
36.564 -7.437 2.328
-7.437 30.812 -1.596
2.328 -1.596 25.133

orbtensor 9 C
-213.530 24.998 -19.139
24.998 -194.198 13.112
-19.139 13.112 -67.068
250.918 3.551 3.620
3.551 253.665 -2.480
3.620 -2.480 233.538

orbtensor 10 H
-8.488 -6.676 -1.846
-6.676 -4.945 -1.421
-1.846 -1.421 -0.316
35.733 7.706 2.237
7.706 31.644 1.721
2.237 1.721 25.134

orbtensor 11 C
-210.734 -25.904 -18.392
-25.904 -196.992 -14.150
-18.392 -14.150 -67.069
251.315 -3.681 3.477
-3.681 253.268 2.676
3.477 2.676 233.538

orbtensor 12 H
-0.914 -3.748 -0.659
-3.748 -12.519 -2.235
-0.659 -2.235 -0.316
26.991 4.325 0.798
4.325 40.386 2.708
0.798 2.708 25.134

orbtensor 13 C
-181.352 -14.541 -6.559
-14.541 -226.374 -22.261
-6.559 -22.261 -67.071
255.491 -2.066 1.240
-2.066 249.093 4.209
1.240 4.209 233.539

orbtensor 14 H
-9.208 6.443 1.922
6.443 -4.224 -1.317
1.922 -1.317 -0.316
36.564 -7.436 -2.329
-7.436 30.812 1.596
-2.329 1.596 25.133

orbtensor 15 C
-213.532 24.994 19.138
24.994 -194.195 -13.125
19.138 -13.125 -67.071
250.918 3.551 -3.619
3.551 253.664 2.482
-3.619 2.482 233.538

orbtensor 16 H
-8.488 -6.677 1.845
-6.677 -4.946 1.420
1.845 1.420 -0.316
35.733 7.706 -2.236
7.706 31.645 -1.720
-2.236 -1.720 25.133

orbtensor 17 C
-210.735 -25.907 18.385

```

-25.907  -196.997   14.133
18.385   14.133   -67.065
251.316   -3.680   -3.477
-3.680   253.269   -2.674
-3.477   -2.674   233.537

```

```

orbtensor 18 H
-1.360    4.360   -0.780
4.360   -12.074    2.193
-0.780    2.193   -0.316
27.506   -5.033    0.945
-5.033   39.872   -2.657
0.945   -2.657   25.133

```

```

orbtensor 19 C
-183.081  16.920   -7.766
16.920 -224.655   21.842
-7.766   21.842  -67.062
255.246   2.404   1.470
2.404  249.339  -4.132
1.470   -4.132  233.536

```

```

orbtensor 20 C
-230.628  -1.467  -23.182
-1.467 -177.106  -0.645
-23.182  -0.645  -67.066
248.490  -0.209   4.384
-0.209  256.095   0.122
4.384    0.122  233.537

```

```

orbtensor 21 H
-13.614  -0.379  -2.327
-0.379   0.179  -0.064
-2.327  -0.064  -0.316
41.649   0.437   2.820
0.437   25.729   0.077
2.820    0.077  25.134

```

```

gtensor (ppt)
-0.146    0.000    0.000
0.000   -0.146    0.000
0.000    0.000   -0.130
-11.659    0.000    0.000
0.000  -11.659   -0.001
0.000   -0.001   -0.935

```

```

zfstensor (cm-1)
-0.864676    0.000001   -0.000014
 0.000001   -0.864622   -0.000088
-0.000014   -0.000088   1.317295

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-49.6203	-796.21867	24862.09065	-41.73612	24820.35453	24024.13586
2	H	2.8463	26.25400	-375.59186	0.33440	-375.25746	-349.00346
3	C	-1.0173	87.77500	533.76564	1.38366	535.14930	622.92430
4	H	2.8463	26.25400	-375.59186	0.33405	-375.25781	-349.00381
5	C	-1.0177	87.77333	533.94053	1.38282	535.32334	623.09668
6	H	2.8463	26.25400	-375.59186	0.33441	-375.25745	-349.00345
7	C	-1.0177	87.77400	533.94053	1.38283	535.32335	623.09735
8	H	2.8467	26.25433	-375.63584	0.33423	-375.30161	-349.04728

9	C	-1.0177	87.77500	533.94053	1.38401	535.32454	623.09954
10	H	2.8470	26.25400	-375.67983	0.33445	-375.34538	-349.09138
11	C	-1.0170	87.77533	533.59075	1.38443	534.97518	622.75051
12	H	2.8460	26.25400	-375.54787	0.33449	-375.21338	-348.95938
13	C	-1.0163	87.77533	533.24096	1.38364	534.62460	622.39993
14	H	2.8467	26.25367	-375.63584	0.33459	-375.30125	-349.04758
15	C	-1.0170	87.77400	533.59075	1.38451	534.97526	622.74926
16	H	2.8467	26.25367	-375.63584	0.33428	-375.30156	-349.04790
17	C	-1.0173	87.77500	533.76564	1.38367	535.14931	622.92431
18	H	2.8460	26.25367	-375.54787	0.33417	-375.21370	-348.96003
19	C	-1.0177	87.77433	533.94053	1.38279	535.32332	623.09765
20	C	-1.0173	87.77400	533.76564	1.38356	535.14920	622.92320
21	H	2.8460	26.25367	-375.54787	0.33410	-375.21377	-348.96011
13C Average		-1.0173	87.77453	533.74815	1.38359	535.13174	622.90627
1H Average		2.8464	26.25390	-375.60066	0.33432	-375.26634	-349.01244

=====
4VCp2-GTO-B3LYP

Temperature: 298

Spin: 1.5

atensor 1 V

5.9976 0.0000 0.0018
0.0000 5.9976 0.0043
0.0018 0.0043 -55.8674
-9.3316 -0.0000 -0.0001
-0.0000 -9.3316 -0.0004
-0.0001 -0.0004 -4.0104

atensor 2 H

0.4309 -1.4182 -1.3091
-1.4182 3.9150 3.6815
-1.3091 3.6815 3.6784
0.0185 0.0064 0.0066
0.0064 0.0027 -0.0186
0.0066 -0.0186 -0.0021

atensor 3 C

-1.6488 -0.2571 -0.6031
-0.2571 -1.0174 1.6963
-0.6031 1.6963 0.6745
0.0490 0.0066 0.0077
0.0066 0.0328 -0.0217
0.0077 -0.0217 0.0005

atensor 4 H

4.4161 0.1233 -3.9058
0.1233 -0.0704 -0.1073
-3.9058 -0.1073 3.6777
0.0005 -0.0006 0.0197
-0.0006 0.0208 0.0005
0.0197 0.0005 -0.0021

atensor 5 C

-0.9261 0.0224 -1.7998
0.0224 -1.7394 -0.0495
-1.7998 -0.0495 0.6748
0.0305 -0.0006 0.0231
-0.0006 0.0513 0.0006
0.0231 0.0006 0.0005

atensor 6 H

0.2853 1.2190 -1.1051
1.2190 4.0596 -3.7476
-1.1051 -3.7476 3.6774
0.0192 -0.0055 0.0056

-0.0055 0.0021 0.0189
0.0056 0.0189 -0.0021

atensor 7 C
-1.6744 0.2210 -0.5092
0.2210 -0.9902 -1.7270
-0.5092 -1.7270 0.6753
0.0497 -0.0056 0.0065
-0.0056 0.0322 0.0221
0.0065 0.0221 0.0005

atensor 8 H
2.9825 -2.0952 3.2227
-2.0952 1.3624 -2.2092
3.2227 -2.2092 3.6781
0.0070 0.0095 -0.0163
0.0095 0.0143 0.0112
-0.0163 0.0112 -0.0021

atensor 9 C
-1.1857 -0.3798 1.4850
-0.3798 -1.4793 -1.0180
1.4850 -1.0180 0.6752
0.0372 0.0097 -0.0190
0.0097 0.0447 0.0130
-0.0190 0.0130 0.0005

atensor 10 H
2.7485 2.1712 3.0969
2.1712 1.5966 2.3825
3.0969 2.3825 3.6786
0.0080 -0.0098 -0.0157
-0.0098 0.0132 -0.0120
-0.0157 -0.0120 -0.0021

atensor 11 C
-1.2286 0.3935 1.4270
0.3935 -1.4374 1.0977
1.4270 1.0977 0.6751
0.0383 -0.0101 -0.0183
-0.0101 0.0436 -0.0141
-0.0183 -0.0141 0.0005

atensor 12 H
0.2856 1.2188 1.1052
1.2188 4.0591 3.7477
1.1052 3.7477 3.6786
0.0192 -0.0055 -0.0056
-0.0055 0.0021 -0.0189
-0.0056 -0.0189 -0.0021

atensor 13 C
-1.6747 0.2209 0.5092
0.2209 -0.9909 1.7267
0.5092 1.7267 0.6753
0.0497 -0.0056 -0.0065
-0.0056 0.0322 -0.0221
-0.0065 -0.0221 0.0005

atensor 14 H
2.9830 -2.0949 -3.2230
-2.0949 1.3622 2.2089
-3.2230 2.2089 3.6789
0.0070 0.0095 0.0163
0.0095 0.0143 -0.0112
0.0163 -0.0112 -0.0021

atensor 15 C
-1.1861 -0.3797 -1.4851
-0.3797 -1.4799 1.0177
-1.4851 1.0177 0.6752
0.0372 0.0097 0.0190
0.0097 0.0447 -0.0130
0.0190 -0.0130 0.0005

atensor 16 H
2.7487 2.1715 -3.0967
2.1715 1.5973 -2.3827
-3.0967 -2.3827 3.6780
0.0080 -0.0098 0.0157
-0.0098 0.0132 0.0120
0.0157 0.0120 -0.0021

atensor 17 C
-1.2284 0.3937 -1.4270
0.3937 -1.4370 -1.0980
-1.4270 -1.0980 0.6746
0.0383 -0.0101 0.0183
-0.0101 0.0436 0.0141
0.0183 0.0141 0.0005

atensor 18 H
0.4302 -1.4184 1.3089
-1.4184 3.9154 -3.6815
1.3089 -3.6815 3.6771
0.0185 0.0064 -0.0066
0.0064 0.0027 0.0186
-0.0066 0.0186 -0.0021

atensor 19 C
-1.6484 -0.2571 0.6031
-0.2571 -1.0166 -1.6966
0.6031 -1.6966 0.6752
0.0490 0.0066 -0.0077
0.0066 0.0328 0.0217
-0.0077 0.0217 0.0005

atensor 20 C
-0.9260 0.0222 1.7997
0.0222 -1.7392 0.0492
1.7997 0.0492 0.6745
0.0305 -0.0006 -0.0231
-0.0006 0.0513 -0.0006
-0.0231 -0.0006 0.0005

atensor 21 H
4.4158 0.1229 3.9058
0.1229 -0.0705 0.1069
3.9058 0.1069 3.6776
0.0005 -0.0006 -0.0197
-0.0006 0.0208 -0.0005
-0.0197 -0.0005 -0.0021

orbtensor 1 V
1692.2384 0.0000 -0.0005
0.0000 1692.2383 -0.0017
-0.0005 -0.0017 1718.4006
-3689.0808 -0.0029 -0.0475
-0.0029 -3689.0775 -0.2811
-0.0475 -0.2811 -274.2340

orbtensor 2 H
24.9643 -5.6172 -0.6110
-5.6172 38.7666 1.7188

-0.6110 1.7188 24.2349
1.6298 5.1920 0.4670
5.1920 -11.1273 -1.3134
0.4670 -1.3134 0.5963

orbtensor 3 C
251.5012 -0.3898 -1.0793
-0.3898 252.4579 3.0391
-1.0793 3.0391 236.7511
-189.9684 21.3441 7.7307
21.3441 -242.4104 -21.7607
7.7307 -21.7607 -78.6411

orbtensor 4 H
40.7506 0.4880 -1.8226
0.4880 22.9807 -0.0502
-1.8226 -0.0502 24.2346
-12.9610 -0.4508 1.3926
-0.4508 3.4633 0.0384
1.3926 0.0384 0.5964

orbtensor 5 C
252.5966 0.0341 -3.2231
0.0341 251.3644 -0.0887
-3.2231 -0.0887 236.7507
-249.9490 -1.8534 23.0767
-1.8534 -182.4273 0.6317
23.0767 0.6317 -78.6374

orbtensor 6 H
24.3911 4.8277 -0.5156
4.8277 39.3406 -1.7490
-0.5156 -1.7490 24.2344
2.1597 -4.4622 0.3940
-4.4622 -11.6573 1.3363
0.3940 1.3363 0.5967

orbtensor 7 C
251.4628 0.3351 -0.9114
0.3351 252.4989 -3.0928
-0.9114 -3.0928 236.7503
-187.7861 -18.3455 6.5255
-18.3455 -244.5907 22.1438
6.5255 22.1438 -78.6370

orbtensor 8 H
35.0752 -8.2990 1.5049
-8.2990 28.6564 -1.0316
1.5049 -1.0316 24.2347
-7.7151 7.6704 -1.1499
7.6704 -1.7824 0.7883
-1.1499 0.7883 0.5966

orbtensor 9 C
252.2026 -0.5752 2.6610
-0.5752 251.7582 -1.8230
2.6610 -1.8230 236.7507
-228.3843 31.5347 -19.0514
31.5347 -203.9945 13.0530
-19.0514 13.0530 -78.6399

orbtensor 10 H
34.1470 8.6005 1.4465
8.6005 29.5840 1.1127
1.4465 1.1127 24.2349
-6.8570 -7.9491 -1.1055
-7.9491 -2.6400 -0.8504

-1.1055 -0.8504 0.5963

orbtensor 11 C

252.1371 0.5961 2.5572
0.5961 251.8212 1.9668
2.5572 1.9668 236.7509
-224.8540 -32.6781 -18.3105
-32.6781 -207.5187 -14.0849
-18.3105 -14.0849 -78.6423

orbtensor 12 H

24.3908 4.8275 0.5162
4.8275 39.3398 1.7506
0.5162 1.7506 24.2350
2.1599 -4.4621 -0.3946
-4.4621 -11.6568 -1.3378
-0.3946 -1.3378 0.5964

orbtensor 13 C

251.4608 0.3349 0.9122
0.3349 252.4963 3.0947
0.9122 3.0947 236.7511
-187.7884 -18.3437 -6.5289
-18.3437 -244.5863 -22.1604
-6.5289 -22.1604 -78.6435

orbtensor 14 H

35.0752 -8.2990 -1.5054
-8.2990 28.6559 1.0319
-1.5054 1.0319 24.2346
-7.7150 7.6704 1.1506
7.6704 -1.7820 -0.7884
1.1506 -0.7884 0.5969

orbtensor 15 C

252.2028 -0.5750 -2.6602
-0.5750 251.7581 1.8248
-2.6602 1.8248 236.7512
-228.3837 31.5322 19.0512
31.5322 -203.9924 -13.0652
19.0512 -13.0652 -78.6428

orbtensor 16 H

34.1473 8.6009 -1.4452
8.6009 29.5844 -1.1118
-1.4452 -1.1118 24.2343
-6.8574 -7.9496 1.1042
-7.9496 -2.6403 0.8498
1.1042 0.8498 0.5973

orbtensor 17 C

252.1396 0.5963 -2.5564
0.5963 251.8238 -1.9650
-2.5564 -1.9650 236.7507
-224.8592 -32.6826 18.3001
-32.6826 -207.5236 14.0678
18.3001 14.0678 -78.6387

orbtensor 18 H

24.9644 -5.6173 0.6105
-5.6173 38.7671 -1.7172
0.6105 -1.7172 24.2344
1.6298 5.1921 -0.4665
5.1921 -11.1276 1.3122
-0.4665 1.3122 0.5971

orbtensor 19 C

251.5023 -0.3898 1.0801
 -0.3898 252.4595 -3.0373
 1.0801 -3.0373 236.7505
 -189.9657 21.3457 -7.7301
 21.3457 -242.4139 21.7419
 -7.7301 21.7419 -78.6360

orbtensor 20 C
 252.5950 0.0337 3.2235
 0.0337 251.3628 0.0904
 3.2235 0.0904 236.7507
 -249.9503 -1.8527 -23.0768
 -1.8527 -182.4283 -0.6422
 -23.0768 -0.6422 -78.6395

orbtensor 21 H
 40.7502 0.4879 1.8227
 0.4879 22.9806 0.0501
 1.8227 0.0501 24.2349
 -12.9609 -0.4509 -1.3929
 -0.4509 3.4633 -0.0380
 -1.3929 -0.0380 0.5965

gtensor (ppt)
 -0.0707 -0.0000 -0.0000
 -0.0000 -0.0707 -0.0000
 -0.0000 -0.0000 -0.0536
 -10.6165 -0.0000 -0.0001
 -0.0000 -10.6165 -0.0009
 -0.0001 -0.0009 -0.9408

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-22.1819	-849.83833	11118.79608	30.60321	11149.39929	10299.56096
2	H	2.6811	26.35487	-353.93997	-0.21264	-354.15261	-327.79774
3	C	-0.6365	76.56343	334.07368	-1.11465	332.95903	409.52246
4	H	2.6809	26.35487	-353.90477	-0.21270	-354.11747	-327.76261
5	C	-0.6361	76.56600	333.89872	-1.11492	332.78380	409.34980
6	H	2.6805	26.35507	-353.85637	-0.21285	-354.06922	-327.71415
7	C	-0.6356	76.56607	333.63627	-1.11516	332.52112	409.08718
8	H	2.6807	26.35513	-353.88717	-0.21287	-354.10004	-327.74490
9	C	-0.6358	76.56427	333.72376	-1.11507	332.60869	409.17295
10	H	2.6809	26.35507	-353.91357	-0.21275	-354.12632	-327.77126
11	C	-0.6362	76.56473	333.91621	-1.11497	332.80125	409.36598
12	H	2.6808	26.35503	-353.90037	-0.21273	-354.11310	-327.75807
13	C	-0.6360	76.56333	333.81124	-1.11488	332.69635	409.25969
14	H	2.6811	26.35520	-353.93557	-0.21282	-354.14839	-327.79319
15	C	-0.6361	76.56440	333.89872	-1.11509	332.78363	409.34803
16	H	2.6810	26.35520	-353.92677	-0.21282	-354.13959	-327.78439
17	C	-0.6361	76.56420	333.89872	-1.11490	332.78381	409.34801
18	H	2.6806	26.35507	-353.86957	-0.21275	-354.08232	-327.72725
19	C	-0.6358	76.56557	333.74125	-1.11522	332.62603	409.19160
20	C	-0.6361	76.56347	333.89872	-1.11459	332.78413	409.34760
21	H	2.6807	26.35487	-353.88277	-0.21268	-354.09544	-327.74058
	ring 1H	2.6808	26.35504	-353.90169	-0.21276	-354.11445	-327.75941
	ring 13C	-0.6360	76.56455	333.84973	-1.11494	332.73478	409.29933

=====
 4VCp2-GTO-BHLYP
 Temperature: 298
 Spin: 1.5

atensor 1 V

-49.8997 0.0001 0.0006
0.0001 -49.8997 0.0037
0.0006 0.0037 -112.4987
-11.6326 0.0000 -0.0001
0.0000 -11.6326 -0.0005
-0.0001 -0.0005 -3.1739

atensor 2 H
0.2195 -1.4134 -1.3387
-1.4134 3.6919 3.7648
-1.3387 3.7648 3.4182
0.0261 0.0112 0.0086
0.0112 -0.0013 -0.0242
0.0086 -0.0242 -0.0014

atensor 3 C
-1.7936 -0.2742 -0.6100
-0.2742 -1.1202 1.7157
-0.6100 1.7157 0.3751
0.0553 0.0072 0.0090
0.0072 0.0376 -0.0253
0.0090 -0.0253 0.0008

atensor 4 H
4.1919 0.1229 -3.9942
0.1229 -0.2792 -0.1097
-3.9942 -0.1097 3.4181
-0.0053 -0.0010 0.0257
-0.0010 0.0300 0.0007
0.0257 0.0007 -0.0014

atensor 5 C
-1.0234 0.0239 -1.8204
0.0239 -1.8908 -0.0501
-1.8204 -0.0501 0.3744
0.0351 -0.0006 0.0269
-0.0006 0.0578 0.0007
0.0269 0.0007 0.0008

atensor 6 H
0.0753 1.2148 -1.1301
1.2148 3.8366 -3.8325
-1.1301 -3.8325 3.4179
0.0272 -0.0096 0.0073
-0.0096 -0.0025 0.0247
0.0073 0.0247 -0.0014

atensor 7 C
-1.8216 0.2357 -0.5150
0.2357 -1.0919 -1.7467
-0.5150 -1.7467 0.3745
0.0560 -0.0062 0.0076
-0.0062 0.0369 0.0258
0.0076 0.0258 0.0008

atensor 8 H
2.7630 -2.0882 3.2956
-2.0882 1.1484 -2.2592
3.2956 -2.2592 3.4184
0.0060 0.0165 -0.0212
0.0165 0.0188 0.0145
-0.0212 0.0145 -0.0014

atensor 9 C
-1.3003 -0.4051 1.5020
-0.4051 -1.6134 -1.0296
1.5020 -1.0296 0.3758

0.0423 0.0106 -0.0222
0.0106 0.0505 0.0152
-0.0222 0.0152 0.0008

atensor 10 H
2.5295 2.1638 3.1670
2.1638 1.3816 2.4364
3.1670 2.4364 3.4186
0.0079 -0.0171 -0.0204
-0.0171 0.0169 -0.0157
-0.0204 -0.0157 -0.0014

atensor 11 C
-1.3457 0.4197 1.4433
0.4197 -1.5683 1.1103
1.4433 1.1103 0.3751
0.0435 -0.0110 -0.0213
-0.0110 0.0494 -0.0164
-0.0213 -0.0164 0.0008

atensor 12 H
0.0752 1.2146 1.1302
1.2146 3.8357 3.8326
1.1302 3.8326 3.4186
0.0272 -0.0096 -0.0073
-0.0096 -0.0025 -0.0247
-0.0073 -0.0247 -0.0014

atensor 13 C
-1.8215 0.2356 0.5150
0.2356 -1.0922 1.7465
0.5150 1.7465 0.3749
0.0560 -0.0062 -0.0076
-0.0062 0.0369 -0.0258
-0.0076 -0.0258 0.0008

atensor 14 H
2.7632 -2.0878 -3.2959
-2.0878 1.1479 2.2589
-3.2959 2.2589 3.4188
0.0060 0.0165 0.0212
0.0165 0.0188 -0.0145
0.0212 -0.0145 -0.0014

atensor 15 C
-1.3002 -0.4049 -1.5021
-0.4049 -1.6136 1.0294
-1.5021 1.0294 0.3760
0.0423 0.0106 0.0222
0.0106 0.0506 -0.0152
0.0222 -0.0152 0.0008

atensor 16 H
2.5297 2.1642 -3.1668
2.1642 1.3822 -2.4366
-3.1668 -2.4366 3.4180
0.0079 -0.0171 0.0204
-0.0171 0.0169 0.0157
0.0204 0.0157 -0.0014

atensor 17 C
-1.3456 0.4199 -1.4433
0.4199 -1.5681 -1.1105
-1.4433 -1.1105 0.3748
0.0435 -0.0110 0.0213
-0.0110 0.0494 0.0164
0.0213 0.0164 0.0008

atensor 18 H

0.2194 -1.4135 1.3385
-1.4135 3.6926 -3.7648
1.3385 -3.7648 3.4173
0.0261 0.0112 -0.0086
0.0112 -0.0013 0.0242
-0.0086 0.0242 -0.0014

atensor 19 C

-1.7935 -0.2742 0.6100
-0.2742 -1.1197 -1.7159
0.6100 -1.7159 0.3749
0.0553 0.0072 -0.0090
0.0072 0.0376 0.0253
-0.0090 0.0253 0.0008

atensor 20 C

-1.0234 0.0237 1.8203
0.0237 -1.8907 0.0498
1.8203 0.0498 0.3744
0.0351 -0.0006 -0.0268
-0.0006 0.0578 -0.0007
-0.0268 -0.0007 0.0008

atensor 21 H

4.1917 0.1225 3.9942
0.1225 -0.2793 0.1093
3.9942 0.1093 3.4182
-0.0053 -0.0010 -0.0257
-0.0010 0.0300 -0.0007
-0.0257 -0.0007 -0.0014

orbtensor 1 V

1691.7199 0.0000 -0.0004
0.0000 1691.7198 -0.0017
-0.0004 -0.0017 1720.1601
-4657.0125 0.0043 -0.0373
0.0043 -4656.9952 -0.2641
-0.0373 -0.2641 -164.4683

orbtensor 2 H

25.0488 -5.6781 -0.5577
-5.6781 39.0007 1.5687
-0.5577 1.5687 24.1495
2.3653 5.5645 0.6062
5.5645 -11.3072 -1.7049
0.6062 -1.7049 0.3925

orbtensor 3 C

252.3657 -0.4012 -1.0545
-0.4012 253.3509 2.9699
-1.0545 2.9699 236.1212
-183.2061 22.6869 8.3562
22.6869 -238.9474 -23.5206
8.3562 -23.5206 -70.6642

orbtensor 4 H

41.0063 0.4932 -1.6634
0.4932 23.0438 -0.0458
-1.6634 -0.0458 24.1493
-13.2728 -0.4832 1.8080
-0.4832 4.3301 0.0498
1.8080 0.0498 0.3927

orbtensor 5 C

253.4940 0.0351 -3.1495

0.0351 252.2252 -0.0866
-3.1495 -0.0866 236.1210
-246.9638 -1.9707 24.9424
-1.9707 -175.1946 0.6824
24.9424 0.6824 -70.6617

orbtensor 6 H
24.4694 4.8800 -0.4705
4.8800 39.5810 -1.5962
-0.4705 -1.5962 24.1491
2.9331 -4.7824 0.5115
-4.7824 -11.8754 1.7348
0.5115 1.7348 0.3930

orbtensor 7 C
252.3263 0.3449 -0.8904
0.3449 253.3931 -3.0222
-0.8904 -3.0222 236.1205
-180.8904 -19.4990 7.0533
-19.4990 -241.2672 23.9347
7.0533 23.9347 -70.6612

orbtensor 8 H
35.2693 -8.3890 1.3736
-8.3890 28.7809 -0.9415
1.3736 -0.9415 24.1493
-7.6501 8.2208 -1.4926
8.2208 -1.2918 1.0232
-1.4926 1.0232 0.3928

orbtensor 9 C
253.0876 -0.5922 2.6004
-0.5922 252.6299 -1.7812
2.6004 -1.7812 236.1209
-224.0381 33.5182 -20.5923
33.5182 -198.1154 14.1087
-20.5923 14.1087 -70.6634

orbtensor 10 H
34.3311 8.6937 1.3203
8.6937 29.7185 1.0155
1.3203 1.0155 24.1496
-6.7306 -8.5195 -1.4347
-8.5195 -2.2108 -1.1036
-1.4347 -1.1036 0.3924

orbtensor 11 C
253.0204 0.6137 2.4990
0.6137 252.6948 1.9218
2.4990 1.9218 236.1212
-220.2876 -34.7343 -19.7900
-34.7343 -201.8606 -15.2231
-19.7900 -15.2231 -70.6658

orbtensor 12 H
24.4691 4.8799 0.4711
4.8799 39.5801 1.5978
0.4711 1.5978 24.1496
2.9334 -4.7822 -0.5121
-4.7822 -11.8746 -1.7361
-0.5121 -1.7361 0.3924

orbtensor 13 C
252.3239 0.3447 0.8911
0.3447 253.3902 3.0242
0.8911 3.0242 236.1213
-180.8882 -19.4980 -7.0570

-19.4980 -241.2600 -23.9515
-7.0570 -23.9515 -70.6665

orbtensor 14 H
35.2693 -8.3889 -1.3741
-8.3889 28.7804 0.9419
-1.3741 0.9419 24.1493
-7.6501 8.2207 1.4931
8.2207 -1.2914 -1.0232
1.4931 -1.0232 0.3928

orbtensor 15 C
253.0880 -0.5920 -2.5997
-0.5920 252.6300 1.7832
-2.5997 1.7832 236.1214
-224.0385 33.5159 20.5915
33.5159 -198.1118 -14.1209
20.5915 -14.1209 -70.6660

orbtensor 16 H
34.3314 8.6941 -1.3190
8.6941 29.7190 -1.0147
-1.3190 -1.0147 24.1490
-6.7309 -8.5200 1.4334
-8.5200 -2.2114 1.1030
1.4334 1.1030 0.3931

orbtensor 17 C
253.0232 0.6139 -2.4981
0.6139 252.6979 -1.9199
-2.4981 -1.9199 236.1209
-220.2907 -34.7374 19.7811
-34.7374 -201.8666 15.2067
19.7811 15.2067 -70.6615

orbtensor 18 H
25.0490 -5.6781 0.5571
-5.6781 39.0012 -1.5671
0.5571 -1.5671 24.1491
2.3651 5.5646 -0.6056
5.5646 -11.3077 1.7035
-0.6056 1.7035 0.3929

orbtensor 19 C
252.3667 -0.4012 1.0552
-0.4012 253.3524 -2.9680
1.0552 -2.9680 236.1206
-183.2063 22.6877 -8.3554
22.6877 -238.9532 23.5008
-8.3554 23.5008 -70.6593

orbtensor 20 C
253.4919 0.0348 3.1499
0.0348 252.2231 0.0885
3.1499 0.0885 236.1210
-246.9612 -1.9686 -24.9436
-1.9686 -175.1922 -0.6938
-24.9436 -0.6938 -70.6625

orbtensor 21 H
41.0058 0.4932 1.6636
0.4932 23.0437 0.0457
1.6636 0.0457 24.1496
-13.2723 -0.4832 -1.8081
-0.4832 4.3302 -0.0494
-1.8081 -0.0494 0.3924

```

gtensor (ppt)
-0.0709  0.0000  -0.0000
0.0000  -0.0709  -0.0000
-0.0000  -0.0000  -0.0518
-16.9733  0.0000  -0.0001
0.0000  -16.9732  -0.0010
-0.0001  -0.0010  -0.5641

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-79.5791	-1458.29207	39807.15334	49.66435	39856.81769	38398.52562
2	H	2.4510	26.54987	-322.89285	-0.34983	-323.24268	-296.69281
3	C	-0.8150	83.00670	426.90193	-1.71564	425.18629	508.19299
4	H	2.4514	26.54980	-322.94115	-0.34984	-323.29099	-296.74119
5	C	-0.8154	83.00670	427.09399	-1.71548	425.37851	508.38521
6	H	2.4510	26.55007	-322.89724	-0.35005	-323.24728	-296.69722
7	C	-0.8151	83.00703	426.95431	-1.71552	425.23879	508.24582
8	H	2.4511	26.55013	-322.90163	-0.35012	-323.25175	-296.70162
9	C	-0.8148	83.00717	426.77971	-1.71675	425.06296	508.07013
10	H	2.4510	26.55007	-322.89724	-0.35000	-323.24724	-296.69717
11	C	-0.8151	83.00747	426.93685	-1.71581	425.22105	508.22851
12	H	2.4509	26.55000	-322.88406	-0.34999	-323.23405	-296.68405
13	C	-0.8150	83.00690	426.91939	-1.71538	425.20401	508.21091
14	H	2.4511	26.55010	-322.90602	-0.35008	-323.25610	-296.70600
15	C	-0.8147	83.00770	426.74479	-1.71664	425.02815	508.03585
16	H	2.4511	26.55007	-322.90602	-0.35000	-323.25602	-296.70595
17	C	-0.8151	83.00773	426.93685	-1.71581	425.22104	508.22878
18	H	2.4509	26.54987	-322.87967	-0.34986	-323.22953	-296.67967
19	C	-0.8149	83.00697	426.83209	-1.71574	425.11635	508.12332
20	C	-0.8153	83.00670	427.07653	-1.71536	425.36118	508.36788
21	H	2.4513	26.54980	-322.93237	-0.34985	-323.28222	-296.73242
	ring 1H	2.4511	26.54998	-322.90382	-0.34996	-323.25379	-296.70381
	ring 13C	-0.8150	83.00711	426.91764	-1.71581	425.20183	508.20894

```

=====
4VCp2-GTO-BP
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
35.8425 0.0001 0.0011
0.0001 35.8426 0.0038
0.0011 0.0038 -22.5734
-7.5312 -0.0000 0.0001
-0.0000 -7.5312 -0.0001
0.0001 -0.0001 -4.3936

```

```

atensor 2 H
0.4942 -1.3933 -1.2777
-1.3933 3.9173 3.5933
-1.2777 3.5933 3.8287
0.0132 0.0030 0.0051
0.0030 0.0057 -0.0145
0.0051 -0.0145 -0.0026

```

```

atensor 3 C
-1.6898 -0.2375 -0.5984
-0.2375 -1.1064 1.6831
-0.5984 1.6831 0.6839
0.0443 0.0061 0.0065
0.0061 0.0294 -0.0184
0.0065 -0.0184 0.0002

```

atensor 4 H
4.4097 0.1211 -3.8122
0.1211 0.0020 -0.1047
-3.8122 -0.1047 3.8281
0.0046 -0.0003 0.0154
-0.0003 0.0142 0.0004
0.0154 0.0004 -0.0026

atensor 5 C
-1.0221 0.0207 -1.7857
0.0207 -1.7735 -0.0491
-1.7857 -0.0491 0.6841
0.0273 -0.0005 0.0195
-0.0005 0.0464 0.0005
0.0195 0.0005 0.0002

atensor 6 H
0.3519 1.1976 -1.0787
1.1976 4.0598 -3.6578
-1.0787 -3.6578 3.8282
0.0135 -0.0026 0.0043
-0.0026 0.0054 0.0147
0.0043 0.0147 -0.0026

atensor 7 C
-1.7139 0.2042 -0.5052
0.2042 -1.0818 -1.7135
-0.5052 -1.7135 0.6841
0.0449 -0.0052 0.0055
-0.0052 0.0288 0.0187
0.0055 0.0187 0.0002

atensor 8 H
3.0016 -2.0584 3.1455
-2.0584 1.4099 -2.1563
3.1455 -2.1563 3.8288
0.0077 0.0045 -0.0127
0.0045 0.0112 0.0087
-0.0127 0.0087 -0.0026

atensor 9 C
-1.2625 -0.3509 1.4734
-0.3509 -1.5337 -1.0100
1.4734 -1.0100 0.6842
0.0334 0.0089 -0.0161
0.0089 0.0403 0.0110
-0.0161 0.0110 0.0002

atensor 10 H
2.7713 2.1331 3.0227
2.1331 1.6396 2.3254
3.0227 2.3254 3.8289
0.0082 -0.0047 -0.0122
-0.0047 0.0107 -0.0094
-0.0122 -0.0094 -0.0026

atensor 11 C
-1.3016 0.3636 1.4159
0.3636 -1.4945 1.0891
1.4159 1.0891 0.6844
0.0344 -0.0093 -0.0155
-0.0093 0.0393 -0.0119
-0.0155 -0.0119 0.0002

atensor 12 H
0.3519 1.1974 1.0787
1.1974 4.0591 3.6579

1.0787 3.6579 3.8292
0.0135 -0.0026 -0.0043
-0.0026 0.0054 -0.0147
-0.0043 -0.0147 -0.0026

atensor 13 C
-1.7143 0.2041 0.5052
0.2041 -1.0824 1.7133
0.5052 1.7133 0.6842
0.0449 -0.0052 -0.0055
-0.0052 0.0288 -0.0187
-0.0055 -0.0187 0.0002

atensor 14 H
3.0015 -2.0582 -3.1457
-2.0582 1.4092 2.1560
-3.1457 2.1560 3.8290
0.0077 0.0045 0.0127
0.0045 0.0112 -0.0087
0.0127 -0.0087 -0.0026

atensor 15 C
-1.2621 -0.3508 -1.4734
-0.3508 -1.5337 1.0098
-1.4734 1.0098 0.6848
0.0334 0.0089 0.0161
0.0089 0.0403 -0.0110
0.0161 -0.0110 0.0002

atensor 16 H
2.7717 2.1334 -3.0225
2.1334 1.6405 -2.3256
-3.0225 -2.3256 3.8286
0.0082 -0.0047 0.0122
-0.0047 0.0107 0.0094
0.0122 0.0094 -0.0026

atensor 17 C
-1.3016 0.3637 -1.4158
0.3637 -1.4943 -1.0893
-1.4158 -1.0893 0.6837
0.0344 -0.0093 0.0155
-0.0093 0.0393 0.0119
0.0155 0.0119 0.0002

atensor 18 H
0.4943 -1.3934 1.2775
-1.3934 3.9181 -3.5933
1.2775 -3.5933 3.8280
0.0132 0.0030 -0.0051
0.0030 0.0057 0.0145
-0.0051 0.0145 -0.0026

atensor 19 C
-1.6898 -0.2376 0.5984
-0.2376 -1.1060 -1.6833
0.5984 -1.6833 0.6836
0.0443 0.0061 -0.0065
0.0061 0.0294 0.0184
-0.0065 0.0184 0.0002

atensor 20 C
-1.0219 0.0205 1.7857
0.0205 -1.7733 0.0489
1.7857 0.0489 0.6844
0.0273 -0.0005 -0.0195
-0.0005 0.0464 -0.0005

-0.0195 -0.0005 0.0002

atensor 21 H

4.4091 0.1207 3.8122
0.1207 0.0015 0.1043
3.8122 0.1043 3.8278
0.0046 -0.0003 -0.0154
-0.0003 0.0142 -0.0004
-0.0154 -0.0004 -0.0026

orbtensor 1 V

1695.3854 0.0000 -0.0001
0.0000 1695.3854 -0.0012
-0.0001 -0.0012 1718.1578
-3082.0891 -0.0022 0.0218
-0.0022 -3082.0910 -0.1182
0.0218 -0.1182 -354.8591

orbtensor 2 H

24.6810 -5.8831 -0.7660
-5.8831 39.1363 2.1548
-0.7660 2.1548 24.0061
1.1105 5.1088 0.4796
5.1088 -11.4418 -1.3488
0.4796 -1.3488 0.7892

orbtensor 3 C

252.5952 -0.0548 -1.0890
-0.0548 252.7285 3.0657
-1.0890 3.0657 238.7266
-191.6347 18.7713 7.2343
18.7713 -237.7521 -20.3651
7.2343 -20.3651 -82.1299

orbtensor 4 H

41.2142 0.5111 -2.2851
0.5111 22.6034 -0.0628
-2.2851 -0.0628 24.0058
-13.2462 -0.4437 1.4303
-0.4437 2.9147 0.0393
1.4303 0.0393 0.7894

orbtensor 5 C

252.7485 0.0049 -3.2515
0.0049 252.5762 -0.0894
-3.2515 -0.0894 238.7263
-244.3841 -1.6308 21.5961
-1.6308 -185.0072 0.5905
21.5961 0.5905 -82.1282

orbtensor 6 H

24.0805 5.0562 -0.6465
5.0562 39.7373 -2.1928
-0.6465 -2.1928 24.0057
1.6319 -4.3907 0.4047
-4.3907 -11.9634 1.3724
0.4047 1.3724 0.7893

orbtensor 7 C

252.5908 0.0471 -0.9196
0.0471 252.7350 -3.1200
-0.9196 -3.1200 238.7259
-189.7214 -16.1325 6.1065
-16.1325 -239.6718 20.7238
6.1065 20.7238 -82.1278

orbtensor 8 H

35.2701 -8.6918 1.8866
-8.6918 28.5476 -1.2932
1.8866 -1.2932 24.0060
-8.0845 7.5474 -1.1809
7.5474 -2.2471 0.8095
-1.1809 0.8095 0.7891

orbtensor 9 C
252.6934 -0.0802 2.6842
-0.0802 252.6321 -1.8391
2.6842 -1.8391 238.7263
-225.4182 27.7314 -17.8301
27.7314 -203.9724 12.2156
-17.8301 12.2156 -82.1289

orbtensor 10 H
34.2981 9.0075 1.8133
9.0075 29.5192 1.3949
1.8133 1.3949 24.0062
-7.2403 -7.8216 -1.1351
-7.8216 -3.0909 -0.8732
-1.1351 -0.8732 0.7890

orbtensor 11 C
252.6835 0.0832 2.5796
0.0832 252.6398 1.9842
2.5796 1.9842 238.7264
-222.3150 -28.7385 -17.1352
-28.7385 -207.0690 -13.1811
-17.1352 -13.1811 -82.1307

orbtensor 12 H
24.0803 5.0560 0.6472
5.0560 39.7366 2.1945
0.6472 2.1945 24.0063
1.6320 -4.3905 -0.4053
-4.3905 -11.9629 -1.3736
-0.4053 -1.3736 0.7889

orbtensor 13 C
252.5891 0.0470 0.9205
0.0470 252.7329 3.1217
0.9205 3.1217 238.7266
-189.7164 -16.1323 -6.1101
-16.1323 -239.6660 -20.7391
-6.1101 -20.7391 -82.1314

orbtensor 14 H
35.2701 -8.6916 -1.8871
-8.6916 28.5471 1.2936
-1.8871 1.2936 24.0059
-8.0844 7.5473 1.1812
7.5473 -2.2466 -0.8097
1.1812 -0.8097 0.7890

orbtensor 15 C
252.6935 -0.0800 -2.6833
-0.0800 252.6318 1.8409
-2.6833 1.8409 238.7268
-225.4192 27.7285 17.8288
27.7285 -203.9686 -12.2278
17.8288 -12.2278 -82.1314

orbtensor 16 H
34.2983 9.0079 -1.8120
9.0079 29.5196 -1.3940
-1.8120 -1.3940 24.0056

-7.2405 -7.8220 1.1339
 -7.8220 -3.0912 0.8727
 1.1339 0.8727 0.7894

orbtensor 17 C
 252.6853 0.0833 -2.5788
 0.0833 252.6417 -1.9825
 -2.5788 -1.9825 238.7263
 -222.3181 -28.7391 17.1277
 -28.7391 -207.0761 13.1657
 17.1277 13.1657 -82.1280

orbtensor 18 H
 24.6810 -5.8831 0.7655
 -5.8831 39.1368 -2.1531
 0.7655 -2.1531 24.0057
 1.1104 5.1088 -0.4792
 5.1088 -11.4422 1.3474
 -0.4792 1.3474 0.7895

orbtensor 19 C
 252.5960 -0.0548 1.0899
 -0.0548 252.7299 -3.0639
 1.0899 -3.0639 238.7261
 -191.6355 18.7709 -7.2344
 18.7709 -237.7580 20.3469
 -7.2344 20.3469 -82.1262

orbtensor 20 C
 252.7473 0.0046 3.2520
 0.0046 252.5750 0.0911
 3.2520 0.0911 238.7262
 -244.3834 -1.6283 -21.5968
 -1.6283 -185.0028 -0.6021
 -21.5968 -0.6021 -82.1285

orbtensor 21 H
 41.2138 0.5109 2.2853
 0.5109 22.6033 0.0627
 2.2853 0.0627 24.0061
 -13.2459 -0.4436 -1.4304
 -0.4436 2.9146 -0.0391
 -1.4304 -0.0391 0.7893

gtensor (ppt)
 -0.0690 -0.0000 -0.0000
 -0.0000 -0.0690 -0.0000
 -0.0000 -0.0000 -0.0524
 -5.9570 -0.0000 0.0001
 -0.0000 -5.9570 -0.0001
 0.0001 -0.0001 -1.2134

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	9.8852	-470.03687	-4962.51256	14.69309	-4947.81947	-5417.85634
2	H	2.7522	26.09377	-363.86665	-0.11274	-363.97940	-337.88563
3	C	-0.6795	77.51120	357.18325	-0.56925	356.61399	434.12519
4	H	2.7520	26.09377	-363.84462	-0.11270	-363.95732	-337.86356
5	C	-0.6792	77.51050	357.04306	-0.56923	356.47383	433.98433
6	H	2.7521	26.09377	-363.85343	-0.11274	-363.96617	-337.87240
7	C	-0.6792	77.51023	357.06059	-0.56930	356.49129	434.00152
8	H	2.7522	26.09373	-363.87106	-0.11280	-363.98386	-337.89012
9	C	-0.6794	77.51077	357.13068	-0.56942	356.56126	434.07203
10	H	2.7520	26.09377	-363.84902	-0.11280	-363.96183	-337.86806

11	C	-0.6793	77.51167	357.07811	-0.56942	356.50869	434.02035
12	H	2.7522	26.09373	-363.86665	-0.11281	-363.97946	-337.88573
13	C	-0.6795	77.51160	357.21829	-0.56942	356.64887	434.16047
14	H	2.7520	26.09370	-363.84462	-0.11279	-363.95741	-337.86371
15	C	-0.6790	77.51097	356.95545	-0.56944	356.38601	433.89697
16	H	2.7524	26.09373	-363.89309	-0.11273	-364.00583	-337.91209
17	C	-0.6794	77.51037	357.16572	-0.56919	356.59654	434.10690
18	H	2.7522	26.09373	-363.87547	-0.11271	-363.98817	-337.89444
19	C	-0.6794	77.51077	357.16572	-0.56919	356.59653	434.10730
20	C	-0.6790	77.51127	356.92040	-0.56932	356.35108	433.86235
21	H	2.7515	26.09373	-363.78292	-0.11275	-363.89567	-337.80194
	ring 1H	2.7521	26.09374	-363.85475	-0.11276	-363.96751	-337.87377
	ring 13C	-0.6793	77.51093	357.09213	-0.56932	356.52281	434.03374

=====
4VCp2-GTO-CAM-B3LYP

Temperature: 298

Spin: 1.5

atensor 2 H

0.3915 -1.4067 -1.3183
-1.4067 3.8475 3.7074
-1.3183 3.7074 3.6194
0.0198 0.0074 0.0068
0.0074 0.0017 -0.0191
0.0068 -0.0191 -0.0017

atensor 3 C

-1.8099 -0.2658 -0.6061
-0.2658 -1.1570 1.7047
-0.6061 1.7047 0.3765
0.0507 0.0068 0.0077
0.0068 0.0341 -0.0218
0.0077 -0.0218 0.0006

orbtensor 2 H

24.8662 -5.6458 -0.6578
-5.6458 38.7392 1.8503
-0.6578 1.8503 24.0972
1.7607 5.2511 0.5346
5.2511 -11.1418 -1.5036
0.5346 -1.5036 0.5043

orbtensor 3 C

251.4417 -0.2895 -1.3386
-0.2895 252.1533 3.7690
-1.3386 3.7690 236.2519
-188.3329 22.3177 8.1561
22.3177 -243.1667 -22.9590
8.1561 -22.9590 -74.3170

gtensor (ppt)

-0.0717 0.0000 0.0000
0.0000 -0.0717 0.0000
0.0000 0.0000 -0.0536
-12.1223 0.0000 -0.0002
0.0000 -12.1224 -0.0005
-0.0002 -0.0005 -0.7253

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
	ring 1H	2.626	26.2753	-346.5085	-0.2496	-346.7581	-320.4828

ring 13C -0.835 78.0101 438.0765 -1.2134 436.8631 514.8732

=====
4Vcp2-GTO-HF
Temperature: 298
Spin: 1.5

atensor 1 V
-167.5865 0.0000 0.0056
0.0000 -167.5864 0.0070
0.0056 0.0070 -222.0990
-14.7606 -0.0000 -0.0007
-0.0000 -14.7606 -0.0012
-0.0007 -0.0012 -1.7354

atensor 2 H
0.1234 -1.3142 -1.3919
-1.3142 3.3520 3.9143
-1.3919 3.9143 3.3475
0.0375 0.0178 0.0117
0.0178 -0.0063 -0.0330
0.0117 -0.0330 -0.0007

atensor 3 C
-2.6735 -0.2850 -0.6101
-0.2850 -1.9735 1.7154
-0.6101 1.7154 -1.1667
0.0680 0.0081 0.0106
0.0081 0.0481 -0.0299
0.0106 -0.0299 0.0010

atensor 4 H
3.8158 0.1143 -4.1527
0.1143 -0.3420 -0.1141
-4.1527 -0.1141 3.3461
-0.0126 -0.0015 0.0350
-0.0015 0.0438 0.0010
0.0350 0.0010 -0.0007

atensor 5 C
-1.8716 0.0248 -1.8201
0.0248 -2.7732 -0.0501
-1.8201 -0.0501 -1.1646
0.0453 -0.0007 0.0318
-0.0007 0.0708 0.0009
0.0318 0.0009 0.0010

atensor 6 H
-0.0116 1.1296 -1.1750
1.1296 3.4860 -3.9845
-1.1750 -3.9845 3.3465
0.0394 -0.0153 0.0099
-0.0153 -0.0081 0.0336
0.0099 0.0336 -0.0007

atensor 7 C
-2.7022 0.2450 -0.5150
0.2450 -1.9438 -1.7465
-0.5150 -1.7465 -1.1656
0.0688 -0.0069 0.0090
-0.0069 0.0473 0.0305
0.0090 0.0305 0.0010

atensor 8 H
2.4879 -1.9415 3.4264
-1.9415 0.9866 -2.3489
3.4264 -2.3489 3.3473

0.0054 0.0264 -0.0289
0.0264 0.0258 0.0198
-0.0289 0.0198 -0.0007

atensor 9 C
-2.1601 -0.4210 1.5016
-0.4210 -2.4856 -1.0296
1.5016 -1.0296 -1.1656
0.0534 0.0119 -0.0262
0.0119 0.0627 0.0180
-0.0262 0.0180 0.0010

atensor 10 H
2.2713 2.0118 3.2927
2.0118 1.2040 2.5331
3.2927 2.5331 3.3480
0.0084 -0.0273 -0.0278
-0.0273 0.0229 -0.0214
-0.0278 -0.0214 -0.0007

atensor 11 C
-2.2079 0.4362 1.4430
0.4362 -2.4393 1.1101
1.4430 1.1101 -1.1665
0.0548 -0.0124 -0.0252
-0.0124 0.0613 -0.0194
-0.0252 -0.0194 0.0010

atensor 12 H
-0.0105 1.1293 1.1751
1.1293 3.4858 3.9847
1.1751 3.9847 3.3482
0.0394 -0.0153 -0.0099
-0.0153 -0.0081 -0.0336
-0.0099 -0.0336 -0.0007

atensor 13 C
-2.7029 0.2449 0.5148
0.2449 -1.9449 1.7463
0.5148 1.7463 -1.1672
0.0688 -0.0069 -0.0090
-0.0069 0.0473 -0.0305
-0.0090 -0.0305 0.0010

atensor 14 H
2.4876 -1.9414 -3.4267
-1.9414 0.9856 2.3485
-3.4267 2.3485 3.3473
0.0054 0.0264 0.0289
0.0264 0.0258 -0.0198
0.0289 -0.0198 -0.0007

atensor 15 C
-2.1597 -0.4209 -1.5019
-0.4209 -2.4854 1.0292
-1.5019 1.0292 -1.1642
0.0534 0.0119 0.0262
0.0119 0.0627 -0.0180
0.0262 -0.0180 0.0010

atensor 16 H
2.2706 2.0124 -3.2924
2.0124 1.2036 -2.5333
-3.2924 -2.5333 3.3466
0.0084 -0.0273 0.0278
-0.0273 0.0229 0.0214
0.0278 0.0214 -0.0007

atensor 17 C
-2.2072 0.4364 -1.4431
0.4364 -2.4384 -1.1103
-1.4431 -1.1103 -1.1652
0.0548 -0.0124 0.0252
-0.0124 0.0613 0.0194
0.0252 0.0194 0.0010

atensor 18 H
0.1228 -1.3144 1.3916
-1.3144 3.3524 -3.9143
1.3916 -3.9143 3.3462
0.0375 0.0178 -0.0117
0.0178 -0.0063 0.0330
-0.0117 0.0330 -0.0007

atensor 19 C
-2.6731 -0.2850 0.6097
-0.2850 -1.9727 -1.7157
0.6097 -1.7157 -1.1659
0.0680 0.0081 -0.0106
0.0081 0.0481 0.0299
-0.0106 0.0299 0.0010

atensor 20 C
-1.8722 0.0246 1.8199
0.0246 -2.7737 0.0498
1.8199 0.0498 -1.1663
0.0453 -0.0007 -0.0318
-0.0007 0.0708 -0.0009
-0.0318 -0.0009 0.0010

atensor 21 H
3.8163 0.1138 4.1528
0.1138 -0.3410 0.1136
4.1528 0.1136 3.3469
-0.0126 -0.0015 -0.0350
-0.0015 0.0438 -0.0010
-0.0350 -0.0010 -0.0007

orbtensor 1 V
1689.7440 0.0001 -0.0012
0.0001 1689.7441 -0.0025
-0.0012 -0.0025 1721.6688
-6454.4403 -0.0047 -0.4161
-0.0047 -6454.4481 -0.6435
-0.4161 -0.6435 -63.9517

orbtensor 2 H
25.6434 -5.8887 -0.4919
-5.8887 40.1131 1.3841
-0.4919 1.3841 24.1735
3.2769 6.2442 0.9106
6.2442 -12.0663 -2.5604
0.9106 -2.5604 0.1402

orbtensor 3 C
256.1289 -0.0423 -0.7049
-0.0423 256.2333 1.9877
-0.7049 1.9877 235.5278
-170.1541 23.5901 9.2647
23.5901 -228.1152 -26.0734
9.2647 -26.0734 -59.2315

orbtensor 4 H
42.1932 0.5115 -1.4674

0.5115 23.5641 -0.0404
-1.4674 -0.0404 24.1733
-14.2713 -0.5421 2.7153
-0.5421 5.4818 0.0749
2.7153 0.0749 0.1411

orbtensor 5 C
256.2500 0.0039 -2.1069
0.0039 256.1158 -0.0579
-2.1069 -0.0579 235.5277
-236.4501 -2.0486 27.6508
-2.0486 -161.8204 0.7576
27.6508 0.7576 -59.2261

orbtensor 6 H
25.0424 5.0611 -0.4151
5.0611 40.7150 -1.4081
-0.4151 -1.4081 24.1731
3.9143 -5.3664 0.7684
-5.3664 -12.7032 2.6053
0.7684 2.6053 0.1415

orbtensor 7 C
256.1263 0.0364 -0.5952
0.0364 256.2389 -2.0220
-0.5952 -2.0220 235.5271
-167.7409 -20.2761 7.8203
-20.2761 -230.5247 26.5336
7.8203 26.5336 -59.2251

orbtensor 8 H
36.2432 -8.7004 1.2118
-8.7004 29.5139 -0.8306
1.2118 -0.8306 24.1733
-7.9622 9.2251 -2.2412
9.2251 -0.8268 1.5366
-2.2412 1.5366 0.1405

orbtensor 9 C
256.2052 -0.0623 1.7405
-0.0623 256.1570 -1.1913
1.7405 -1.1913 235.5272
-212.6114 34.8529 -22.8268
34.8529 -185.6552 15.6415
-22.8268 15.6415 -59.2299

orbtensor 10 H
35.2700 9.0164 1.1649
9.0164 30.4862 0.8960
1.1649 0.8960 24.1736
-6.9304 -9.5605 -2.1544
-9.5605 -1.8584 -1.6573
-2.1544 -1.6573 0.1397

orbtensor 11 C
256.1971 0.0644 1.6725
0.0644 256.1625 1.2859
1.6725 1.2859 235.5277
-208.7110 -36.1162 -21.9380
-36.1162 -189.5507 -16.8757
-21.9380 -16.8757 -59.2342

orbtensor 12 H
25.0420 5.0609 0.4157
5.0609 40.7140 1.4098
0.4157 1.4098 24.1736
3.9142 -5.3667 -0.7687

-5.3667 -12.7027 -2.6070
-0.7687 -2.6070 0.1395

orbtensor 13 C
256.1232 0.0364 0.5958
0.0364 256.2353 2.0244
0.5958 2.0244 235.5276
-167.7446 -20.2743 -7.8227
-20.2743 -230.5172 -26.5511
-7.8227 -26.5511 -59.2340

orbtensor 14 H
36.2432 -8.7004 -1.2125
-8.7004 29.5135 0.8311
-1.2125 0.8311 24.1732
-7.9616 9.2249 2.2421
9.2249 -0.8265 -1.5362
2.2421 -1.5362 0.1409

orbtensor 15 C
256.2058 -0.0621 -1.7397
-0.0621 256.1576 1.1937
-1.7397 1.1937 235.5277
-212.6085 34.8515 22.8274
34.8515 -185.6493 -15.6522
22.8274 -15.6522 -59.2313

orbtensor 16 H
35.2706 9.0168 -1.1636
9.0168 30.4869 -0.8951
-1.1636 -0.8951 24.1731
-6.9302 -9.5606 2.1527
-9.5606 -1.8587 1.6566
2.1527 1.6566 0.1419

orbtensor 17 C
256.2006 0.0645 -1.6716
0.0645 256.1663 -1.2835
-1.6716 -1.2835 235.5275
-208.7129 -36.1235 21.9281
-36.1235 -189.5541 16.8585
21.9281 16.8585 -59.2259

orbtensor 18 H
25.6435 -5.8888 0.4914
-5.8888 40.1135 -1.3823
0.4914 -1.3823 24.1732
3.2766 6.2445 -0.9095
6.2445 -12.0662 2.5590
-0.9095 2.5590 0.1412

orbtensor 19 C
256.1301 -0.0423 0.7055
-0.0423 256.2345 -1.9853
0.7055 -1.9853 235.5273
-170.1523 23.5923 -9.2620
23.5923 -228.1191 26.0543
-9.2620 26.0543 -59.2245

orbtensor 20 C
256.2472 0.0038 2.1073
0.0038 256.1130 0.0602
2.1073 0.0602 235.5277
-236.4469 -2.0470 -27.6524
-2.0470 -161.8237 -0.7674
-27.6524 -0.7674 -59.2301

```

orbtensor 21 H
42.1925 0.5115 1.4675
0.5115 23.5638 0.0404
1.4675 0.0404 24.1736
-14.2715 -0.5423 -2.7157
-0.5423 5.4818 -0.0741
-2.7157 -0.0741 0.1396

```

```

gtensor (ppt)
-0.0783 0.0000 -0.0000
0.0000 -0.0783 -0.0000
-0.0000 -0.0000 -0.0465
-26.4031 -0.0000 -0.0018
-0.0000 -26.4032 -0.0027
-0.0018 -0.0027 -0.2475

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-196.1762	-2623.89440	97826.67587	60.66549	97887.34136	95263.44696
2	H	2.2845	27.09360	-300.01897	-0.61331	-300.63227	-273.53867
3	C	-1.8989	96.79640	991.54802	-1.68333	989.86469	1086.66109
4	H	2.2835	27.09407	-299.88764	-0.61378	-300.50141	-273.40735
5	C	-1.8974	96.79897	990.79957	-1.68607	989.11350	1085.91246
6	H	2.2838	27.09437	-299.93579	-0.61401	-300.54980	-273.45544
7	C	-1.8982	96.80053	991.18250	-1.68583	989.49666	1086.29720
8	H	2.2841	27.09397	-299.97081	-0.61377	-300.58458	-273.49061
9	C	-1.8981	96.79763	991.13028	-1.68465	989.44563	1086.24326
10	H	2.2846	27.09357	-300.04085	-0.61330	-300.65415	-273.56059
11	C	-1.8989	96.79713	991.54802	-1.68344	989.86458	1086.66171
12	H	2.2847	27.09353	-300.04961	-0.61337	-300.66298	-273.56944
13	C	-1.8993	96.79677	991.77430	-1.68282	990.09148	1086.88825
14	H	2.2837	27.09423	-299.91390	-0.61400	-300.52791	-273.43367
15	C	-1.8974	96.80067	990.78216	-1.68631	989.09585	1085.89652
16	H	2.2838	27.09453	-299.93141	-0.61409	-300.54550	-273.45097
17	C	-1.8979	96.80050	991.04325	-1.68614	989.35711	1086.15761
18	H	2.2840	27.09393	-299.95330	-0.61355	-300.56685	-273.47292
19	C	-1.8982	96.79867	991.19990	-1.68486	989.51504	1086.31371
20	C	-1.8984	96.79573	991.28693	-1.68313	989.60380	1086.39953
21	H	2.2842	27.09327	-299.98832	-0.61312	-300.60144	-273.50817
	ring 1H	2.2841	27.09391	-299.96906	-0.61363	-300.58269	-273.48878
	ring 13C	-1.8983	96.79830	991.22949	-1.68466	989.54483	1086.34313

```

=====
4VCp2-GTO-LC-PBE0
Temperature: 298
Spin: 1.5

```

```

atensor 2 H
0.2785 -1.3485 -1.3322
-1.3485 3.5910 3.7466
-1.3322 3.7466 3.5333
0.0213 0.0082 0.0072
0.0082 0.0011 -0.0201
0.0072 -0.0201 -0.0015

```

```

atensor 3 C
-2.1323 -0.2701 -0.6040
-0.2701 -1.4688 1.6984
-0.6040 1.6984 -0.3516
0.0533 0.0072 0.0079
0.0072 0.0357 -0.0223
0.0079 -0.0223 0.0008

```



```

orbtensor 2 H
24.6056 -6.0156 -0.8013
-6.0156 39.3868 2.2540
-0.8013 2.2540 23.6555
1.7237 5.4558 0.6529
5.4558 -11.6815 -1.8364
0.6529 -1.8364 0.4457

```

```

orbtensor 3 C
252.6741 0.0227 -1.4120
0.0227 252.6187 3.9758
-1.4120 3.9758 237.0515
-184.5913 21.4720 8.2252
21.4720 -237.3466 -23.1537
8.2252 -23.1537 -68.7362

```

```

gtensor (ppt)
-0.0729 0.0000 0.0000
0.0000 -0.0729 0.0000
0.0000 0.0000 -0.0520
-13.3124 -0.0001 -0.0005
-0.0001 -13.3127 -0.0003
-0.0005 -0.0003 -0.6039

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
ring 1H		2.475	26.0453	-326.3947	-0.2968	-326.6916	-300.6463
ring 13C		-1.288	83.8901	675.2920	-1.0459	674.2461	758.1362

```

====
4VCp2-GTO-PBE
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
25.8428 0.0000 0.0004
0.0000 25.8429 0.0029
0.0004 0.0029 -31.6315
-7.4950 -0.0000 -0.0000
-0.0000 -7.4951 -0.0002
-0.0000 -0.0002 -4.2768

```

```

atensor 2 H
0.5143 -1.3910 -1.2811
-1.3910 3.9316 3.6026
-1.2811 3.6026 3.8458
0.0133 0.0031 0.0052
0.0031 0.0056 -0.0146
0.0052 -0.0146 -0.0026

```

```

atensor 3 C
-1.8009 -0.2389 -0.5929
-0.2389 -1.2141 1.6676
-0.5929 1.6676 0.5714
0.0444 0.0061 0.0066
0.0061 0.0293 -0.0185
0.0066 -0.0185 0.0002

```

```

atensor 4 H
4.4230 0.1209 -3.8221
0.1209 0.0226 -0.1050
-3.8221 -0.1050 3.8450
0.0045 -0.0003 0.0155

```

-0.0003 0.0144 0.0004
0.0155 0.0004 -0.0026

atensor 5 C
-1.1293 0.0208 -1.7693
0.0208 -1.8851 -0.0486
-1.7693 -0.0486 0.5716
0.0271 -0.0005 0.0197
-0.0005 0.0465 0.0005
0.0197 0.0005 0.0002

atensor 6 H
0.3714 1.1957 -1.0815
1.1957 4.0734 -3.6674
-1.0815 -3.6674 3.8448
0.0136 -0.0027 0.0044
-0.0027 0.0052 0.0149
0.0044 0.0149 -0.0026

atensor 7 C
-1.8250 0.2054 -0.5006
0.2054 -1.1892 -1.6977
-0.5006 -1.6977 0.5723
0.0450 -0.0053 0.0056
-0.0053 0.0286 0.0189
0.0056 0.0189 0.0002

atensor 8 H
3.0171 -2.0550 3.1537
-2.0550 1.4280 -2.1619
3.1537 -2.1619 3.8457
0.0076 0.0046 -0.0128
0.0046 0.0112 0.0088
-0.0128 0.0088 -0.0026

atensor 9 C
-1.3712 -0.3529 1.4598
-0.3529 -1.6439 -1.0007
1.4598 -1.0007 0.5719
0.0333 0.0091 -0.0162
0.0091 0.0403 0.0111
-0.0162 0.0111 0.0002

atensor 10 H
2.7874 2.1295 3.0306
2.1295 1.6576 2.3315
3.0306 2.3315 3.8459
0.0081 -0.0048 -0.0123
-0.0048 0.0107 -0.0095
-0.0123 -0.0095 -0.0026

atensor 11 C
-1.4103 0.3657 1.4028
0.3657 -1.6043 1.0791
1.4028 1.0791 0.5722
0.0343 -0.0094 -0.0156
-0.0094 0.0393 -0.0120
-0.0156 -0.0120 0.0002

atensor 12 H
0.3716 1.1954 1.0816
1.1954 4.0727 3.6674
1.0816 3.6674 3.8458
0.0136 -0.0027 -0.0044
-0.0027 0.0052 -0.0149
-0.0044 -0.0149 -0.0026

atensor 13 C
-1.8251 0.2053 0.5005
0.2053 -1.1896 1.6975
0.5005 1.6975 0.5722
0.0450 -0.0053 -0.0056
-0.0053 0.0286 -0.0189
-0.0056 -0.0189 0.0002

atensor 14 H
3.0172 -2.0547 -3.1539
-2.0547 1.4275 2.1616
-3.1539 2.1616 3.8460
0.0076 0.0046 0.0128
0.0046 0.0112 -0.0088
0.0128 -0.0088 -0.0026

atensor 15 C
-1.3709 -0.3528 -1.4599
-0.3528 -1.6440 1.0005
-1.4599 1.0005 0.5721
0.0333 0.0091 0.0162
0.0091 0.0403 -0.0111
0.0162 -0.0111 0.0002

atensor 16 H
2.7875 2.1299 -3.0303
2.1299 1.6582 -2.3317
-3.0303 -2.3317 3.8454
0.0081 -0.0048 0.0123
-0.0048 0.0107 0.0095
0.0123 0.0095 -0.0026

atensor 17 C
-1.4104 0.3658 -1.4028
0.3658 -1.6042 -1.0793
-1.4028 -1.0793 0.5716
0.0343 -0.0094 0.0156
-0.0094 0.0393 0.0120
0.0156 0.0120 0.0002

atensor 18 H
0.5140 -1.3911 1.2808
-1.3911 3.9321 -3.6026
1.2808 -3.6026 3.8448
0.0133 0.0031 -0.0052
0.0031 0.0056 0.0146
-0.0052 0.0146 -0.0026

atensor 19 C
-1.8008 -0.2389 0.5928
-0.2389 -1.2136 -1.6678
0.5928 -1.6678 0.5711
0.0444 0.0061 -0.0066
0.0061 0.0293 0.0185
-0.0066 0.0185 0.0002

atensor 20 C
-1.1294 0.0206 1.7692
0.0206 -1.8851 0.0484
1.7692 0.0484 0.5716
0.0271 -0.0005 -0.0197
-0.0005 0.0465 -0.0005
-0.0197 -0.0005 0.0002

atensor 21 H
4.4227 0.1205 3.8222
0.1205 0.0225 0.1046

3.8222 0.1046 3.8451
0.0045 -0.0003 -0.0155
-0.0003 0.0144 -0.0004
-0.0155 -0.0004 -0.0026

orbtensor 1 V
1695.4877 0.0000 -0.0002
0.0000 1695.4876 -0.0012
-0.0002 -0.0012 1717.8508
-3075.5294 -0.0001 -0.0269
-0.0001 -3075.5296 -0.1575
-0.0269 -0.1575 -354.3907

orbtensor 2 H
24.5405 -5.6262 -0.7055
-5.6262 38.3646 1.9845
-0.7055 1.9845 24.0871
1.1496 4.8430 0.4184
4.8430 -10.7498 -1.1770
0.4184 -1.1770 0.6134

orbtensor 3 C
248.8398 -0.3331 -1.4762
-0.3331 249.6565 4.1544
-1.4762 4.1544 236.7515
-187.6499 19.1029 7.6380
19.1029 -234.5840 -21.4990
7.6380 -21.4990 -79.9430

orbtensor 4 H
40.3517 0.4887 -2.1045
0.4887 22.5536 -0.0579
-2.1045 -0.0579 24.0867
-12.4603 -0.4206 1.2482
-0.4206 2.8600 0.0346
1.2482 0.0346 0.6140

orbtensor 5 C
249.7750 0.0290 -4.4067
0.0290 248.7223 -0.1212
-4.4067 -0.1212 236.7511
-241.3343 -1.6595 22.7986
-1.6595 -180.9037 0.6232
22.7986 0.6232 -79.9415

orbtensor 6 H
23.9663 4.8354 -0.5955
4.8354 38.9394 -2.0195
-0.5955 -2.0195 24.0866
1.6439 -4.1623 0.3532
-4.1623 -11.2442 1.1983
0.3532 1.1983 0.6150

orbtensor 7 C
248.8073 0.2865 -1.2465
0.2865 249.6919 -4.2284
-1.2465 -4.2284 236.7511
-185.7027 -16.4189 6.4471
-16.4189 -236.5415 21.8766
6.4471 21.8766 -79.9441

orbtensor 8 H
34.6673 -8.3122 1.7376
-8.3122 28.2384 -1.1911
1.7376 -1.1911 24.0869
-7.5670 7.1548 -1.0312
7.1548 -2.0333 0.7071

-1.0312 0.7071 0.6150

orbtensor 9 C

249.4392 -0.4912 3.6372
-0.4912 249.0600 -2.4924
3.6372 -2.4924 236.7518
-222.0364 28.2234 -18.8215
28.2234 -200.2091 12.8953
-18.8215 12.8953 -79.9467

orbtensor 10 H

33.7377 8.6141 1.6701
8.6141 29.1675 1.2847
1.6701 1.2847 24.0872
-6.7668 -7.4148 -0.9912
-7.4148 -2.8332 -0.7621
-0.9912 -0.7621 0.6140

orbtensor 11 C

249.3829 0.5091 3.4954
0.5091 249.1136 2.6887
3.4954 2.6887 236.7517
-218.8762 -29.2469 -18.0882
-29.2469 -203.3601 -13.9149
-18.0882 -13.9149 -79.9467

orbtensor 12 H

23.9661 4.8352 0.5961
4.8352 38.9387 2.0211
0.5961 2.0211 24.0873
1.6437 -4.1618 -0.3535
-4.1618 -11.2429 -1.1989
-0.3535 -1.1989 0.6121

orbtensor 13 C

248.8053 0.2862 1.2473
0.2862 249.6894 4.2299
1.2473 4.2299 236.7519
-185.6959 -16.4173 -6.4516
-16.4173 -236.5278 -21.8955
-6.4516 -21.8955 -79.9449

orbtensor 14 H

34.6673 -8.3121 -1.7381
-8.3121 28.2378 1.1914
-1.7381 1.1914 24.0869
-7.5665 7.1541 1.0309
7.1541 -2.0328 -0.7067
1.0309 -0.7067 0.6125

orbtensor 15 C

249.4389 -0.4911 -3.6364
-0.4911 249.0590 2.4940
-3.6364 2.4940 236.7522
-222.0286 28.2202 18.8233
28.2202 -200.1990 -12.9090
18.8233 -12.9090 -79.9446

orbtensor 16 H

33.7378 8.6145 -1.6688
8.6145 29.1678 -1.2839
-1.6688 -1.2839 24.0866
-6.7665 -7.4145 0.9894
-7.4145 -2.8333 0.7611
0.9894 0.7611 0.6121

orbtensor 17 C

249.3843 0.5096 -3.4947
 0.5096 249.1150 -2.6873
 -3.4947 -2.6873 236.7511
 -218.8707 -29.2485 18.0833
 -29.2485 -203.3578 13.9017
 18.0833 13.9017 -79.9385

orbtensor 18 H
 24.5406 -5.6262 0.7050
 -5.6262 38.3651 -1.9829
 0.7050 -1.9829 24.0867
 1.1493 4.8426 -0.4178
 4.8426 -10.7494 1.1751
 -0.4178 1.1751 0.6114

orbtensor 19 C
 248.8402 -0.3332 1.4771
 -0.3332 249.6580 -4.1529
 1.4771 -4.1529 236.7506
 -187.6449 19.1031 -7.6388
 19.1031 -234.5821 21.4839
 -7.6388 21.4839 -79.9352

orbtensor 20 C
 249.7737 0.0286 4.4071
 0.0286 248.7210 0.1227
 4.4071 0.1227 236.7509
 -241.3256 -1.6576 -22.8031
 -1.6576 -180.8977 -0.6345
 -22.8031 -0.6345 -79.9389

orbtensor 21 H
 40.3514 0.4886 2.1047
 0.4886 22.5537 0.0578
 2.1047 0.0578 24.0872
 -12.4591 -0.4205 -1.2477
 -0.4205 2.8595 -0.0343
 -1.2477 -0.0343 0.6114

gtensor (ppt)
 -0.0726 0.0000 -0.0000
 0.0000 -0.0726 -0.0000
 -0.0000 -0.0000 -0.0524
 -6.0684 -0.0000 -0.0000
 -0.0000 -6.0684 -0.0003
 -0.0000 -0.0003 -1.2142

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	0.2624	-465.54120	-131.73979	14.76735	-116.97244	-582.51364
2	H	2.7693	26.00180	-366.12218	-0.11542	-366.23759	-340.23579
3	C	-0.7899	77.69030	415.22005	-0.58198	414.63807	492.32837
4	H	2.7690	26.00190	-366.07370	-0.11542	-366.18912	-340.18722
5	C	-0.7897	77.68963	415.09739	-0.58205	414.51534	492.20497
6	H	2.7686	26.00233	-366.02522	-0.11548	-366.14071	-340.13838
7	C	-0.7894	77.68733	414.93969	-0.58231	414.35738	492.04472
8	H	2.7690	26.00243	-366.07811	-0.11552	-366.19362	-340.19119
9	C	-0.7898	77.68627	415.16748	-0.58229	414.58519	492.27146
10	H	2.7690	26.00213	-366.08251	-0.11548	-366.19799	-340.19586
11	C	-0.7895	77.68840	415.02730	-0.58219	414.44511	492.13351
12	H	2.7688	26.00167	-366.04726	-0.11548	-366.16274	-340.16107
13	C	-0.7896	77.69267	415.04483	-0.58218	414.46265	492.15532
14	H	2.7690	26.00173	-366.07370	-0.11550	-366.18920	-340.18746
15	C	-0.7897	77.69263	415.09739	-0.58221	414.51518	492.20781

16	H	2.7691	26.00150	-366.09133	-0.11548	-366.20680	-340.20530
17	C	-0.7897	77.69447	415.13244	-0.58213	414.55030	492.24477
18	H	2.7691	26.00123	-366.08692	-0.11543	-366.20235	-340.20112
19	C	-0.7898	77.69553	415.16748	-0.58198	414.58550	492.28103
20	C	-0.7897	77.69447	415.11491	-0.58206	414.53285	492.22732
21	H	2.7689	26.00137	-366.06048	-0.11544	-366.17592	-340.17455
	ring 1H	2.7690	26.00181	-366.07414	-0.11546	-366.18960	-340.18779
	ring 13C	-0.7897	77.69117	415.10090	-0.58214	414.51876	492.20993

=====
 4VCp2-GTO-PBE0
 Temperature: 298
 Spin: 1.5

atensor 1 V
 -25.3147 -0.0000 0.0001
 -0.0000 -25.3146 0.0042
 0.0001 0.0042 -83.9584
 -9.3294 -0.0000 0.0000
 -0.0000 -9.3294 -0.0005
 0.0000 -0.0005 -3.8096

atensor 2 H
 0.3908 -1.3593 -1.3216
 -1.3593 3.7301 3.7168
 -1.3216 3.7168 3.6669
 0.0189 0.0067 0.0067
 0.0067 0.0025 -0.0190
 0.0067 -0.0190 -0.0021

atensor 3 C
 -1.9278 -0.2571 -0.5982
 -0.2571 -1.2963 1.6825
 -0.5982 1.6825 -0.0248
 0.0493 0.0066 0.0078
 0.0066 0.0330 -0.0218
 0.0078 -0.0218 0.0007

atensor 4 H
 4.2105 0.1182 -3.9432
 0.1182 -0.0895 -0.1083
 -3.9432 -0.1083 3.6664
 0.0001 -0.0006 0.0201
 -0.0006 0.0213 0.0006
 0.0201 0.0006 -0.0021

atensor 5 C
 -1.2053 0.0224 -1.7851
 0.0224 -2.0186 -0.0491
 -1.7851 -0.0491 -0.0243
 0.0307 -0.0006 0.0232
 -0.0006 0.0517 0.0006
 0.0232 0.0006 0.0007

atensor 6 H
 0.2516 1.1683 -1.1157
 1.1683 3.8690 -3.7835
 -1.1157 -3.7835 3.6663
 0.0196 -0.0057 0.0057
 -0.0057 0.0018 0.0193
 0.0057 0.0193 -0.0021

atensor 7 C
 -1.9539 0.2210 -0.5050
 0.2210 -1.2696 -1.7130
 -0.5050 -1.7130 -0.0241

0.0500 -0.0057 0.0066
-0.0057 0.0324 0.0222
0.0066 0.0222 0.0007

atensor 8 H
2.8366 -2.0081 3.2535
-2.0081 1.2838 -2.2304
3.2535 -2.2304 3.6670
0.0069 0.0099 -0.0166
0.0099 0.0145 0.0114
-0.0166 0.0114 -0.0021

atensor 9 C
-1.4651 -0.3798 1.4729
-0.3798 -1.7587 -1.0098
1.4729 -1.0098 -0.0240
0.0374 0.0098 -0.0191
0.0098 0.0450 0.0131
-0.0191 0.0131 0.0007

atensor 10 H
2.6121 2.0809 3.1266
2.0809 1.5081 2.4053
3.1266 2.4053 3.6673
0.0080 -0.0102 -0.0160
-0.0102 0.0134 -0.0123
-0.0160 -0.0123 -0.0021

atensor 11 C
-1.5076 0.3935 1.4154
0.3935 -1.7164 1.0887
1.4154 1.0887 -0.0238
0.0385 -0.0101 -0.0184
-0.0101 0.0439 -0.0141
-0.0184 -0.0141 0.0007

atensor 12 H
0.2517 1.1681 1.1158
1.1681 3.8682 3.7836
1.1158 3.7836 3.6672
0.0196 -0.0057 -0.0057
-0.0057 0.0018 -0.0193
-0.0057 -0.0193 -0.0021

atensor 13 C
-1.9539 0.2209 0.5050
0.2209 -1.2701 1.7127
0.5050 1.7127 -0.0240
0.0500 -0.0057 -0.0066
-0.0057 0.0324 -0.0222
-0.0066 -0.0222 0.0007

atensor 14 H
2.8368 -2.0078 -3.2538
-2.0078 1.2834 2.2301
-3.2538 2.2301 3.6674
0.0069 0.0099 0.0166
0.0099 0.0145 -0.0114
0.0166 -0.0114 -0.0021

atensor 15 C
-1.4651 -0.3797 -1.4729
-0.3797 -1.7589 1.0094
-1.4729 1.0094 -0.0240
0.0374 0.0098 0.0191
0.0098 0.0450 -0.0131
0.0191 -0.0131 0.0007


```

atensor 16 H
2.6122 2.0813 -3.1263
2.0813 1.5087 -2.4055
-3.1263 -2.4055 3.6666
0.0080 -0.0102 0.0160
-0.0102 0.0134 0.0123
0.0160 0.0123 -0.0021

atensor 17 C
-1.5075 0.3937 -1.4153
0.3937 -1.7161 -1.0890
-1.4153 -1.0890 -0.0242
0.0385 -0.0101 0.0184
-0.0101 0.0439 0.0141
0.0184 0.0141 0.0007

atensor 18 H
0.3905 -1.3594 1.3214
-1.3594 3.7307 -3.7167
1.3214 -3.7167 3.6661
0.0189 0.0067 -0.0067
0.0067 0.0025 0.0190
-0.0067 0.0190 -0.0021

atensor 19 C
-1.9278 -0.2572 0.5982
-0.2572 -1.2959 -1.6827
0.5982 -1.6827 -0.0246
0.0493 0.0066 -0.0078
0.0066 0.0330 0.0219
-0.0078 0.0219 0.0007

atensor 20 C
-1.2051 0.0222 1.7851
0.0222 -2.0184 0.0488
1.7851 0.0488 -0.0240
0.0307 -0.0006 -0.0232
-0.0006 0.0517 -0.0006
-0.0232 -0.0006 0.0007

atensor 21 H
4.2101 0.1178 3.9432
0.1178 -0.0898 0.1079
3.9432 0.1079 3.6663
0.0001 -0.0006 -0.0201
-0.0006 0.0213 -0.0006
-0.0201 -0.0006 -0.0021

orbtensor 1 V
1695.2750 0.0000 -0.0002
0.0000 1695.2750 -0.0016
-0.0002 -0.0016 1719.4617
-3604.3409 -0.0002 0.0206
-0.0002 -3604.3455 -0.2915
0.0206 -0.2915 -247.3056

orbtensor 2 H
24.7123 -5.7695 -0.6920
-5.7695 38.8887 1.9465
-0.6920 1.9465 23.9771
1.5112 5.1137 0.4887
5.1137 -11.0534 -1.3744
0.4887 -1.3744 0.4849

orbtensor 3 C
250.5727 -0.2590 -1.3699

```

-0.2590 251.2077 3.8561
-1.3699 3.8561 236.6509
-183.8209 20.2405 7.8486
20.2405 -233.5502 -22.0924
7.8486 -22.0924 -73.3903

orbtensor 4 H
40.9265 0.5012 -2.0642
0.5012 22.6749 -0.0568
-2.0642 -0.0568 23.9768
-12.8595 -0.4441 1.4574
-0.4441 3.3171 0.0402
1.4574 0.0402 0.4853

orbtensor 5 C
251.3002 0.0227 -4.0900
0.0227 250.4818 -0.1125
-4.0900 -0.1125 236.6505
-240.7019 -1.7576 23.4280
-1.7576 -176.6718 0.6411
23.4280 0.6411 -73.3875

orbtensor 6 H
24.1235 4.9586 -0.5840
4.9586 39.4783 -1.9808
-0.5840 -1.9808 23.9765
2.0332 -4.3950 0.4123
-4.3950 -11.5755 1.3986
0.4123 1.3986 0.4859

orbtensor 7 C
250.5478 0.2227 -1.1567
0.2227 251.2355 -3.9245
-1.1567 -3.9245 236.6503
-181.7526 -17.3977 6.6246
-17.3977 -235.6207 22.4807
6.6246 22.4807 -73.3875

orbtensor 8 H
35.0973 -8.5241 1.7043
-8.5241 28.5044 -1.1683
1.7043 -1.1683 23.9768
-7.6926 7.5548 -1.2034
7.5548 -1.8494 0.8250
-1.2034 0.8250 0.4858

orbtensor 9 C
251.0386 -0.3818 3.3760
-0.3818 250.7439 -2.3131
3.3760 -2.3131 236.6508
-220.2506 29.9053 -19.3409
29.9053 -197.1214 13.2514
-19.3409 13.2514 -73.3899

orbtensor 10 H
34.1439 8.8336 1.6382
8.8336 29.4572 1.2601
1.6382 1.2601 23.9771
-6.8476 -7.8293 -1.1568
-7.8293 -2.6941 -0.8898
-1.1568 -0.8898 0.4852

orbtensor 11 C
250.9947 0.3956 3.2444
0.3956 250.7851 2.4954
3.2444 2.4954 236.6509
-216.9030 -30.9894 -18.5883

-30.9894 -200.4639 -14.2986
-18.5883 -14.2986 -73.3920

orbtensor 12 H
24.1233 4.9584 0.5846
4.9584 39.4775 1.9825
0.5846 1.9825 23.9772
2.0333 -4.3947 -0.4129
-4.3947 -11.5748 -1.3998
-0.4129 -1.3998 0.4848

orbtensor 13 C
250.5457 0.2224 1.1574
0.2224 251.2327 3.9262
1.1574 3.9262 236.6511
-181.7524 -17.3949 -6.6288
-17.3949 -235.6137 -22.4974
-6.6288 -22.4974 -73.3926

orbtensor 14 H
35.0973 -8.5239 -1.7049
-8.5239 28.5039 1.1686
-1.7049 1.1686 23.9768
-7.6926 7.5546 1.2039
7.5546 -1.8491 -0.8250
1.2039 -0.8250 0.4853

orbtensor 15 C
251.0387 -0.3815 -3.3753
-0.3815 250.7435 2.3148
-3.3753 2.3148 236.6514
-220.2503 29.9014 19.3409
29.9014 -197.1200 -13.2638
19.3409 -13.2638 -73.3927

orbtensor 16 H
34.1442 8.8341 -1.6368
8.8341 29.4576 -1.2593
-1.6368 -1.2593 23.9765
-6.8479 -7.8296 1.1555
-7.8296 -2.6944 0.8893
1.1555 0.8893 0.4858

orbtensor 17 C
250.9970 0.3959 -3.2436
0.3959 250.7876 -2.4939
-3.2436 -2.4939 236.6506
-216.9069 -30.9925 18.5794
-30.9925 -200.4675 14.2831
18.5794 14.2831 -73.3879

orbtensor 18 H
24.7124 -5.7696 0.6915
-5.7696 38.8893 -1.9449
0.6915 -1.9449 23.9766
1.5112 5.1137 -0.4881
5.1137 -11.0536 1.3731
-0.4881 1.3731 0.4856

orbtensor 19 C
250.5737 -0.2590 1.3707
-0.2590 251.2096 -3.8544
1.3707 -3.8544 236.6502
-183.8170 20.2425 -7.8482
20.2425 -233.5552 22.0732
-7.8482 22.0732 -73.3850

```

orbtensor 20 C
251.2988 0.0223 4.0904
0.0223 250.4804 0.1141
4.0904 0.1141 236.6504
-240.6998 -1.7569 -23.4289
-1.7569 -176.6682 -0.6519
-23.4289 -0.6519 -73.3878

```

```

orbtensor 21 H
40.9262 0.5011 2.0644
0.5011 22.6749 0.0567
2.0644 0.0567 23.9771
-12.8591 -0.4441 -1.4574
-0.4441 3.3171 -0.0397
-1.4574 -0.0397 0.4850

```

```

gtensor (ppt)
-0.0734 -0.0000 -0.0000
-0.0000 -0.0734 -0.0000
-0.0000 -0.0000 -0.0510
-10.9803 -0.0000 0.0001
-0.0000 -10.9803 -0.0010
0.0001 -0.0010 -0.8596

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-52.3520	-781.99343	26238.85077	30.08804	26268.93880	25486.94537
2	H	2.6024	26.17360	-343.50461	-0.23754	-343.74216	-317.56856
3	C	-1.0553	82.55663	553.85416	-0.91707	552.93709	635.49372
4	H	2.6022	26.17370	-343.48701	-0.23762	-343.72463	-317.55093
5	C	-1.0550	82.55710	553.71421	-0.91756	552.79665	635.35375
6	H	2.6021	26.17397	-343.46501	-0.23781	-343.70282	-317.52885
7	C	-1.0548	82.55760	553.60924	-0.91787	552.69137	635.24897
8	H	2.6022	26.17410	-343.48701	-0.23788	-343.72489	-317.55079
9	C	-1.0549	82.55713	553.64423	-0.91793	552.72630	635.28343
10	H	2.6023	26.17390	-343.49141	-0.23773	-343.72914	-317.55524
11	C	-1.0549	82.55727	553.64423	-0.91774	552.72649	635.28375
12	H	2.6021	26.17377	-343.47381	-0.23767	-343.71148	-317.53772
13	C	-1.0550	82.55693	553.67922	-0.91750	552.76172	635.31865
14	H	2.6023	26.17387	-343.49581	-0.23773	-343.73354	-317.55967
15	C	-1.0550	82.55687	553.67922	-0.91759	552.76163	635.31850
16	H	2.6023	26.17393	-343.49141	-0.23776	-343.72917	-317.55524
17	C	-1.0549	82.55763	553.64423	-0.91771	552.72651	635.28415
18	H	2.6022	26.17383	-343.48261	-0.23774	-343.72035	-317.54652
19	C	-1.0551	82.55877	553.74919	-0.91767	552.83152	635.39029
20	C	-1.0548	82.55793	553.59175	-0.91766	552.67408	635.23202
21	H	2.6020	26.17373	-343.45181	-0.23768	-343.68949	-317.51576
	ring 1H	2.6022	26.17384	-343.48305	-0.23771	-343.72077	-317.54693
	ring 13C	-1.0550	82.55739	553.68097	-0.91763	552.76334	635.32072

```

=====
6MnCp2-STO-B3LYP-No-ZFS
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-87.640 0.000 -0.001
0.000 -87.639 0.000
-0.001 0.000 -85.004
-4.109 0.000 0.000
0.000 -4.109 0.000
0.000 0.000 -4.553

```

atensor 2 H
-2.295 -1.474 -1.210
-1.474 1.329 3.404
-1.210 3.404 0.897
0.000 0.000 0.000
0.000 0.000 0.001
0.000 0.000 0.000

atensor 3 C
-0.081 -0.257 -0.626
-0.257 0.550 1.760
-0.626 1.760 4.188
0.001 -0.002 -0.001
-0.002 0.005 0.002
0.001 -0.003 -0.001

atensor 4 H
1.849 0.128 -3.611
0.128 -2.815 -0.099
-3.611 -0.099 0.897
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.641 0.022 -1.868
0.022 -0.171 -0.051
-1.868 -0.051 4.189
0.005 0.000 -0.002
0.000 0.000 0.000
0.003 0.000 -0.001

atensor 6 H
-2.444 1.268 -1.022
1.268 1.480 -3.465
-1.022 -3.465 0.899
0.000 0.000 0.000
0.000 0.000 -0.001
0.000 0.000 0.000

atensor 7 C
-0.107 0.221 -0.529
0.221 0.575 -1.792
-0.529 -1.792 4.187
0.001 0.001 0.000
0.001 0.005 -0.002
0.001 0.003 -0.001

atensor 8 H
0.361 -2.179 2.980
-2.179 -1.323 -2.043
2.980 -2.043 0.900
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.380 -0.379 1.541
-0.379 0.087 -1.056
1.541 -1.056 4.185
0.004 -0.002 0.001
-0.002 0.002 -0.001
-0.003 0.002 -0.001

atensor 10 H
0.118 2.258 2.864
2.258 -1.081 2.203

2.864 2.203 0.899
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.338 0.393 1.481
0.393 0.130 1.139
1.481 1.139 4.185
0.004 0.002 0.001
0.002 0.002 0.001
-0.002 -0.002 -0.001

atensor 12 H
-2.443 1.267 1.022
1.267 1.481 3.466
1.022 3.466 0.900
0.000 0.000 0.000
0.000 0.000 0.001
0.000 0.000 0.000

atensor 13 C
-0.108 0.220 0.528
0.220 0.575 1.792
0.528 1.792 4.185
0.001 0.001 0.000
0.001 0.005 0.002
-0.001 -0.003 -0.001

atensor 14 H
0.360 -2.178 -2.980
-2.178 -1.326 2.042
-2.980 2.042 0.898
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.381 -0.379 -1.541
-0.379 0.087 1.055
-1.541 1.055 4.189
0.004 -0.002 -0.001
-0.002 0.002 0.001
0.003 -0.002 -0.001

atensor 16 H
0.115 2.258 -2.863
2.258 -1.081 -2.203
-2.863 -2.203 0.896
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.339 0.393 -1.480
0.393 0.131 -1.140
-1.480 -1.140 4.189
0.004 0.002 -0.001
0.002 0.002 -0.001
0.002 0.002 -0.001

atensor 18 H
-2.293 -1.475 1.210
-1.475 1.330 -3.404
1.210 -3.404 0.897
0.000 0.000 0.000
0.000 0.000 -0.001

0.000 0.000 0.000

atensor 19 C
-0.081 -0.257 0.626
-0.257 0.550 -1.761
0.626 -1.761 4.186
0.001 -0.002 0.001
-0.002 0.005 -0.002
-0.001 0.003 -0.001

atensor 20 C
0.640 0.022 1.868
0.022 -0.172 0.051
1.868 0.051 4.184
0.005 0.000 0.002
0.000 0.000 0.000
-0.003 0.000 -0.001

atensor 21 H
1.852 0.128 3.612
0.128 -2.813 0.099
3.612 0.099 0.900
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2027.355 -0.015 0.226
-0.015 -2027.393 -0.109
0.226 -0.109 -109.750
1922.830 0.000 0.002
0.000 1922.831 0.000
0.002 0.000 1930.388

orbtensor 2 H
-1.844 5.736 0.694
5.736 -15.942 -1.953
0.694 -1.953 -0.304
28.380 -4.937 -0.884
-4.937 40.513 2.485
-0.884 2.485 25.406

orbtensor 3 C
-213.174 17.786 5.376
17.786 -256.888 -15.107
5.376 -15.107 -71.937
257.867 2.180 -0.997
2.180 252.507 2.800
-0.997 2.800 233.328

orbtensor 4 H
-17.967 -0.497 2.072
-0.497 0.181 0.057
2.072 0.057 -0.304
42.256 0.428 -2.637
0.428 26.637 -0.072
-2.637 -0.072 25.405

orbtensor 5 C
-263.168 -1.540 16.032
-1.540 -206.895 0.438
16.032 0.438 -71.937
251.738 -0.189 -2.971
-0.189 258.637 -0.081
-2.971 -0.081 233.327

orbtensor 6 H

-1.260	-4.932	0.586
-4.932	-16.525	1.988
0.586	1.988	-0.304
27.877	4.245	-0.746
4.245	41.016	-2.530
-0.746	-2.530	25.405

orbtensor 7 C

-211.356	-15.292	4.540
-15.292	-258.687	15.375
4.540	15.375	-71.935
258.088	-1.875	-0.843
-1.875	252.284	-2.850
-0.843	-2.850	233.328

orbtensor 8 H

-12.169	8.476	-1.708
8.476	-5.616	1.171
-1.708	1.171	-0.304
37.267	-7.295	2.175
-7.295	31.627	-1.491
2.175	-1.491	25.405

orbtensor 9 C

-245.169	26.278	-13.214
26.278	-224.855	9.062
-13.214	9.062	-71.935
253.939	3.223	2.450
3.223	256.431	-1.681
2.450	-1.681	233.328

orbtensor 10 H

-11.224	-8.783	-1.642
-8.783	-6.562	-1.263
-1.642	-1.263	-0.304
36.453	7.560	2.090
7.560	32.440	1.608
2.090	1.608	25.405

orbtensor 11 C

-242.245	-27.233	-12.700
-27.233	-227.794	-9.772
-12.700	-9.772	-71.936
254.299	-3.339	2.354
-3.339	256.072	1.813
2.354	1.813	233.328

orbtensor 12 H

-1.258	-4.929	-0.586
-4.929	-16.526	-1.989
-0.586	-1.989	-0.304
27.876	4.242	0.746
4.242	41.017	2.532
0.746	2.532	25.406

orbtensor 13 C

-211.345	-15.281	-4.521
-15.281	-258.683	-15.394
-4.521	-15.394	-71.938
258.088	-1.874	0.836
-1.874	252.282	2.853
0.836	2.853	233.329

orbtensor 14 H

-12.172	8.475	1.711
8.475	-5.613	-1.173
1.711	-1.173	-0.305

37.269	-7.294	-2.178
-7.294	31.624	1.492
-2.178	1.492	25.406

orbtensor 15 C

-245.197	26.277	13.243
26.277	-224.858	-9.081
13.243	-9.081	-71.940
253.940	3.222	-2.454
3.222	256.433	1.682
-2.454	1.682	233.327

orbtensor 16 H

-11.222	-8.784	1.642
-8.784	-6.565	1.264
1.642	1.264	-0.304
36.451	7.560	-2.091
7.560	32.443	-1.608
-2.091	-1.608	25.405

orbtensor 17 C

-242.254	-27.239	12.719
-27.239	-227.815	9.762
12.719	9.762	-71.937
254.302	-3.339	-2.358
-3.339	256.073	-1.809
-2.358	-1.809	233.327

orbtensor 18 H

-1.845	5.738	-0.694
5.738	-15.941	1.950
-0.694	1.950	-0.304
28.381	-4.938	0.882
-4.938	40.513	-2.483
0.882	-2.483	25.405

orbtensor 19 C

-213.173	17.790	-5.356
17.790	-256.879	15.082
-5.356	15.082	-71.932
257.865	2.181	0.992
2.181	252.508	-2.798
0.992	-2.798	233.327

orbtensor 20 C

-263.144	-1.547	-16.005
-1.547	-206.881	-0.456
-16.005	-0.456	-71.933
251.735	-0.190	2.968
-0.190	258.635	0.085
2.968	0.085	233.328

orbtensor 21 H

-17.966	-0.499	-2.070
-0.499	0.181	-0.057
-2.070	-0.057	-0.304
42.256	0.430	2.635
0.430	26.637	0.073
2.635	0.073	25.405

gtensor (ppt)

-0.142	0.000	0.000
0.000	-0.142	0.000
0.000	0.000	-0.165
0.147	0.000	0.000
0.000	0.147	0.000
0.000	0.000	-0.099

averaging

13C Average:3,5,7,9,11,13,15,17,19,20

1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-91.0180	537.18367	86560.40484	0.06222	86560.46706	87097.65073
2	H	-0.0230	25.40300	5.43337	0.00973	5.44310	30.84610
3	C	1.5540	67.23433	-1459.65109	0.11076	-1459.54033	-1392.30600
4	H	-0.0230	25.40267	5.43337	0.00973	5.44310	30.84577
5	C	1.5543	67.23400	-1459.96418	0.11078	-1459.85340	-1392.61940
6	H	-0.0217	25.40300	5.11839	0.00974	5.12813	30.53113
7	C	1.5533	67.24067	-1459.02490	0.11074	-1458.91416	-1391.67349
8	H	-0.0207	25.40333	4.88215	0.00974	4.89189	30.29523
9	C	1.5523	67.24633	-1458.08561	0.11070	-1457.97491	-1390.72858
10	H	-0.0213	25.40267	5.03964	0.00974	5.04938	30.45205
11	C	1.5527	67.24133	-1458.39871	0.11069	-1458.28802	-1391.04669
12	H	-0.0207	25.40367	4.88215	0.00974	4.89189	30.29556
13	C	1.5523	67.24433	-1458.08561	0.11070	-1457.97491	-1390.73058
14	H	-0.0227	25.40300	5.35462	0.00974	5.36436	30.76736
15	C	1.5540	67.23500	-1459.65109	0.11080	-1459.54029	-1392.30529
16	H	-0.0233	25.40267	5.51211	0.00973	5.52184	30.92450
17	C	1.5547	67.23200	-1460.27728	0.11077	-1460.16651	-1392.93451
18	H	-0.0220	25.40300	5.19713	0.00972	5.20685	30.60985
19	C	1.5533	67.23867	-1459.02490	0.11070	-1458.91420	-1391.67553
20	C	1.5520	67.24667	-1457.77252	0.11067	-1457.66184	-1390.41518
21	H	-0.0203	25.40300	4.80341	0.00974	4.81315	30.21615
13C Average		1.5533	67.23933	-1458.99359	0.11073	-1458.88286	-1391.64352
1H Average		-0.0219	25.40300	5.16563	0.00973	5.17537	30.57837

6MnCp2-STO-B3LYP-ORCA

Temperature: 390

Spin: 2.5

atensor 1 Mn

-87.640 0.000 -0.001
0.000 -87.639 0.000
-0.001 0.000 -85.004
-4.109 0.000 0.000
0.000 -4.109 0.000
0.000 0.000 -4.553

atensor 2 H

-2.295 -1.474 -1.210
-1.474 1.329 3.404
-1.210 3.404 0.897
0.000 0.000 0.000
0.000 0.000 0.001
0.000 0.000 0.000

atensor 3 C

-0.081 -0.257 -0.626
-0.257 0.550 1.760
-0.626 1.760 4.188
0.001 -0.002 -0.001
-0.002 0.005 0.002
0.001 -0.003 -0.001

atensor 4 H

1.849 0.128 -3.611
0.128 -2.815 -0.099
-3.611 -0.099 0.897

0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.641 0.022 -1.868
0.022 -0.171 -0.051
-1.868 -0.051 4.189
0.005 0.000 -0.002
0.000 0.000 0.000
0.003 0.000 -0.001

atensor 6 H
-2.444 1.268 -1.022
1.268 1.480 -3.465
-1.022 -3.465 0.899
0.000 0.000 0.000
0.000 0.000 -0.001
0.000 0.000 0.000

atensor 7 C
-0.107 0.221 -0.529
0.221 0.575 -1.792
-0.529 -1.792 4.187
0.001 0.001 0.000
0.001 0.005 -0.002
0.001 0.003 -0.001

atensor 8 H
0.361 -2.179 2.980
-2.179 -1.323 -2.043
2.980 -2.043 0.900
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.380 -0.379 1.541
-0.379 0.087 -1.056
1.541 -1.056 4.185
0.004 -0.002 0.001
-0.002 0.002 -0.001
-0.003 0.002 -0.001

atensor 10 H
0.118 2.258 2.864
2.258 -1.081 2.203
2.864 2.203 0.899
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.338 0.393 1.481
0.393 0.130 1.139
1.481 1.139 4.185
0.004 0.002 0.001
0.002 0.002 0.001
-0.002 -0.002 -0.001

atensor 12 H
-2.443 1.267 1.022
1.267 1.481 3.466
1.022 3.466 0.900
0.000 0.000 0.000
0.000 0.000 0.001
0.000 0.000 0.000

atensor 13 C
-0.108 0.220 0.528
0.220 0.575 1.792
0.528 1.792 4.185
0.001 0.001 0.000
0.001 0.005 0.002
-0.001 -0.003 -0.001

atensor 14 H
0.360 -2.178 -2.980
-2.178 -1.326 2.042
-2.980 2.042 0.898
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.381 -0.379 -1.541
-0.379 0.087 1.055
-1.541 1.055 4.189
0.004 -0.002 -0.001
-0.002 0.002 0.001
0.003 -0.002 -0.001

atensor 16 H
0.115 2.258 -2.863
2.258 -1.081 -2.203
-2.863 -2.203 0.896
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.339 0.393 -1.480
0.393 0.131 -1.140
-1.480 -1.140 4.189
0.004 0.002 -0.001
0.002 0.002 -0.001
0.002 0.002 -0.001

atensor 18 H
-2.293 -1.475 1.210
-1.475 1.330 -3.404
1.210 -3.404 0.897
0.000 0.000 0.000
0.000 0.000 -0.001
0.000 0.000 0.000

atensor 19 C
-0.081 -0.257 0.626
-0.257 0.550 -1.761
0.626 -1.761 4.186
0.001 -0.002 0.001
-0.002 0.005 -0.002
-0.001 0.003 -0.001

atensor 20 C
0.640 0.022 1.868
0.022 -0.172 0.051
1.868 0.051 4.184
0.005 0.000 0.002
0.000 0.000 0.000
-0.003 0.000 -0.001

atensor 21 H
1.852 0.128 3.612

0.128 -2.813 0.099
3.612 0.099 0.900
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2027.355 -0.015 0.226
-0.015 -2027.393 -0.109
0.226 -0.109 -109.750
1922.830 0.000 0.002
0.000 1922.831 0.000
0.002 0.000 1930.388

orbtensor 2 H
-1.844 5.736 0.694
5.736 -15.942 -1.953
0.694 -1.953 -0.304
28.380 -4.937 -0.884
-4.937 40.513 2.485
-0.884 2.485 25.406

orbtensor 3 C
-213.174 17.786 5.376
17.786 -256.888 -15.107
5.376 -15.107 -71.937
257.867 2.180 -0.997
2.180 252.507 2.800
-0.997 2.800 233.328

orbtensor 4 H
-17.967 -0.497 2.072
-0.497 0.181 0.057
2.072 0.057 -0.304
42.256 0.428 -2.637
0.428 26.637 -0.072
-2.637 -0.072 25.405

orbtensor 5 C
-263.168 -1.540 16.032
-1.540 -206.895 0.438
16.032 0.438 -71.937
251.738 -0.189 -2.971
-0.189 258.637 -0.081
-2.971 -0.081 233.327

orbtensor 6 H
-1.260 -4.932 0.586
-4.932 -16.525 1.988
0.586 1.988 -0.304
27.877 4.245 -0.746
4.245 41.016 -2.530
-0.746 -2.530 25.405

orbtensor 7 C
-211.356 -15.292 4.540
-15.292 -258.687 15.375
4.540 15.375 -71.935
258.088 -1.875 -0.843
-1.875 252.284 -2.850
-0.843 -2.850 233.328

orbtensor 8 H
-12.169 8.476 -1.708
8.476 -5.616 1.171
-1.708 1.171 -0.304
37.267 -7.295 2.175

-7.295 31.627 -1.491
2.175 -1.491 25.405

orbtensor 9 C
-245.169 26.278 -13.214
26.278 -224.855 9.062
-13.214 9.062 -71.935
253.939 3.223 2.450
3.223 256.431 -1.681
2.450 -1.681 233.328

orbtensor 10 H
-11.224 -8.783 -1.642
-8.783 -6.562 -1.263
-1.642 -1.263 -0.304
36.453 7.560 2.090
7.560 32.440 1.608
2.090 1.608 25.405

orbtensor 11 C
-242.245 -27.233 -12.700
-27.233 -227.794 -9.772
-12.700 -9.772 -71.936
254.299 -3.339 2.354
-3.339 256.072 1.813
2.354 1.813 233.328

orbtensor 12 H
-1.258 -4.929 -0.586
-4.929 -16.526 -1.989
-0.586 -1.989 -0.304
27.876 4.242 0.746
4.242 41.017 2.532
0.746 2.532 25.406

orbtensor 13 C
-211.345 -15.281 -4.521
-15.281 -258.683 -15.394
-4.521 -15.394 -71.938
258.088 -1.874 0.836
-1.874 252.282 2.853
0.836 2.853 233.329

orbtensor 14 H
-12.172 8.475 1.711
8.475 -5.613 -1.173
1.711 -1.173 -0.305
37.269 -7.294 -2.178
-7.294 31.624 1.492
-2.178 1.492 25.406

orbtensor 15 C
-245.197 26.277 13.243
26.277 -224.858 -9.081
13.243 -9.081 -71.940
253.940 3.222 -2.454
3.222 256.433 1.682
-2.454 1.682 233.327

orbtensor 16 H
-11.222 -8.784 1.642
-8.784 -6.565 1.264
1.642 1.264 -0.304
36.451 7.560 -2.091
7.560 32.443 -1.608
-2.091 -1.608 25.405

orbtensor 17 C
 -242.254 -27.239 12.719
 -27.239 -227.815 9.762
 12.719 9.762 -71.937
 254.302 -3.339 -2.358
 -3.339 256.073 -1.809
 -2.358 -1.809 233.327

orbtensor 18 H
 -1.845 5.738 -0.694
 5.738 -15.941 1.950
 -0.694 1.950 -0.304
 28.381 -4.938 0.882
 -4.938 40.513 -2.483
 0.882 -2.483 25.405

orbtensor 19 C
 -213.173 17.790 -5.356
 17.790 -256.879 15.082
 -5.356 15.082 -71.932
 257.865 2.181 0.992
 2.181 252.508 -2.798
 0.992 -2.798 233.327

orbtensor 20 C
 -263.144 -1.547 -16.005
 -1.547 -206.881 -0.456
 -16.005 -0.456 -71.933
 251.735 -0.190 2.968
 -0.190 258.635 0.085
 2.968 0.085 233.328

orbtensor 21 H
 -17.966 -0.499 -2.070
 -0.499 0.181 -0.057
 -2.070 -0.057 -0.304
 42.256 0.430 2.635
 0.430 26.637 0.073
 2.635 0.073 25.405

gtensor (ppt)
 -0.142 0.000 0.000
 0.000 -0.142 0.000
 0.000 0.000 -0.165
 0.147 0.000 0.000
 0.000 0.147 0.000
 0.000 0.000 -0.099

zfstensor (cm-1)
 2.395349 0.300375 0.001070
 0.300375 -1.227210 -0.000166
 0.001070 -0.000166 -0.932609

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-91.0180	537.18367	86555.19239	-8.13348	86547.05891	87084.24258
2	H	-0.0230	25.40300	5.43304	-8.14860	-2.71556	22.68744
3	C	1.5540	67.23433	-1459.56319	-19.26293	-1478.82612	-1411.59179
4	H	-0.0230	25.40267	5.43304	6.58776	12.02080	37.42346
5	C	1.5543	67.23400	-1459.87627	-9.00565	-1468.88191	-1401.64791
6	H	-0.0217	25.40300	5.11808	-7.12839	-2.01031	23.39269

7	C	1.5533	67.24067	-1458.93704	-18.53460	-1477.47164	-1410.23097
8	H	-0.0207	25.40333	4.88186	0.34106	5.22292	30.62625
9	C	1.5523	67.24633	-1457.99781	-13.32380	-1471.32161	-1404.07527
10	H	-0.0213	25.40267	5.03934	1.98891	7.02825	32.43092
11	C	1.5527	67.24133	-1458.31088	-12.17970	-1470.49059	-1403.24925
12	H	-0.0207	25.40367	4.88186	-7.12712	-2.24526	23.15841
13	C	1.5523	67.24433	-1457.99781	-18.53421	-1476.53202	-1409.28769
14	H	-0.0227	25.40300	5.35430	0.33191	5.68621	31.08921
15	C	1.5540	67.23500	-1459.56319	-13.35678	-1472.91997	-1405.68497
16	H	-0.0233	25.40267	5.51178	1.97539	7.48717	32.88984
17	C	1.5547	67.23200	-1460.18934	-12.21101	-1472.40035	-1405.16835
18	H	-0.0220	25.40300	5.19682	-8.13917	-2.94235	22.46065
19	C	1.5533	67.23867	-1458.93704	-19.24135	-1478.17839	-1410.93972
20	C	1.5520	67.24667	-1457.68473	-8.96185	-1466.64659	-1399.39992
21	H	-0.0203	25.40300	4.80312	6.60314	11.40626	36.80926
13C Average		1.5533	67.23933	-1458.90573	-14.46119	-1473.36692	-1406.12759
1H Average		-0.0219	25.40300	5.16532	-1.27151	3.89381	29.29681

=====
6Mn Cp2-STO-BHLYP-No-ZFS
Temperature: 390
Spin: 2.5

atensor 1 Mn
-148.584 0.000 0.001
0.000 -148.583 0.000
0.001 0.000 -139.835
-3.816 0.000 0.000
0.000 -3.816 0.000
0.000 0.000 -3.840

atensor 2 H
-2.322 -1.445 -1.237
-1.445 1.231 3.481
-1.237 3.481 0.866
0.001 0.001 0.000
0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 3 C
0.112 -0.275 -0.631
-0.275 0.787 1.776
-0.631 1.776 3.971
-0.001 -0.001 0.000
-0.001 0.001 0.000
0.001 -0.002 0.000

atensor 4 H
1.741 0.125 -3.693
0.125 -2.833 -0.101
-3.693 -0.101 0.865
-0.002 0.000 0.001
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C
0.885 0.024 -1.884
0.024 0.015 -0.051
-1.884 -0.051 3.972
0.001 0.000 -0.001
0.000 -0.002 0.000
0.002 0.000 0.000

atensor 6 H
-2.468 1.243 -1.045
1.243 1.379 -3.544

-1.045 -3.544 0.867
0.001 -0.001 0.000
-0.001 -0.001 0.001
0.000 0.001 0.000

atensor 7 C
0.083 0.236 -0.534
0.236 0.815 -1.808
-0.534 -1.808 3.970
-0.002 0.001 0.000
0.001 0.001 0.000
0.001 0.002 0.000

atensor 8 H
0.282 -2.136 3.048
-2.136 -1.370 -2.089
3.048 -2.089 0.868
-0.001 0.001 -0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 9 C
0.605 -0.406 1.555
-0.406 0.291 -1.066
1.555 -1.066 3.968
0.000 -0.002 0.000
-0.002 -0.001 0.000
-0.002 0.001 0.000

atensor 10 H
0.043 2.214 2.928
2.214 -1.132 2.253
2.928 2.253 0.867
0.000 -0.001 -0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 11 C
0.560 0.421 1.494
0.421 0.337 1.150
1.494 1.150 3.968
0.000 0.002 0.000
0.002 -0.001 0.000
-0.002 -0.001 0.000

atensor 12 H
-2.468 1.242 1.045
1.242 1.379 3.544
1.045 3.544 0.868
0.001 -0.001 0.000
-0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 13 C
0.083 0.236 0.533
0.236 0.814 1.808
0.533 1.808 3.969
-0.002 0.001 0.000
0.001 0.001 0.000
-0.001 -0.002 0.000

atensor 14 H
0.281 -2.135 -3.048
-2.135 -1.373 2.088
-3.048 2.088 0.867
-0.001 0.001 0.001
0.001 0.000 -0.001

0.000 0.000 0.000

atensor 15 C
0.606 -0.406 -1.555
-0.406 0.292 1.065
-1.555 1.065 3.971
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.002 -0.001 0.000

atensor 16 H
0.041 2.214 -2.927
2.214 -1.132 -2.253
-2.927 -2.253 0.865
0.000 -0.001 0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 17 C
0.561 0.421 -1.494
0.421 0.339 -1.150
-1.494 -1.150 3.972
0.000 0.002 0.000
0.002 -0.001 0.000
0.002 0.001 0.000

atensor 18 H
-2.321 -1.446 1.238
-1.446 1.232 -3.481
1.238 -3.481 0.866
0.001 0.001 0.000
0.001 -0.001 0.001
0.000 0.001 0.000

atensor 19 C
0.111 -0.275 0.631
-0.275 0.787 -1.777
0.631 -1.777 3.969
-0.001 -0.001 0.000
-0.001 0.001 0.000
-0.001 0.002 0.000

atensor 20 C
0.883 0.024 1.885
0.024 0.014 0.051
1.885 0.051 3.968
0.001 0.000 0.000
0.000 -0.002 0.000
-0.002 0.000 0.000

atensor 21 H
1.743 0.125 3.694
0.125 -2.831 0.101
3.694 0.101 0.868
-0.002 0.000 -0.001
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1234.995 -0.006 0.177
-0.006 -1235.004 -0.067
0.177 -0.067 -61.163
1922.996 0.000 0.001
0.000 1922.996 0.000
0.001 0.000 1929.676

orbtensor 2 H

-2.308	5.167	0.579
5.167	-15.008	-1.629
0.579	-1.629	-0.573
28.505	-4.828	-0.892
-4.828	40.373	2.510
-0.892	2.510	25.479

orbtensor 3 C

-208.972	17.922	5.407
17.922	-253.023	-15.197
5.407	-15.197	-64.738
258.069	2.852	-1.027
2.852	251.058	2.882
-1.027	2.882	232.468

orbtensor 4 H

-16.832	-0.448	1.728
-0.448	-0.483	0.047
1.728	0.047	-0.574
42.078	0.418	-2.663
0.418	26.801	-0.073
-2.663	-0.073	25.479

orbtensor 5 C

-259.350	-1.552	16.129
-1.552	-202.643	0.441
16.129	0.441	-64.738
250.051	-0.247	-3.059
-0.247	259.076	-0.084
-3.059	-0.084	232.468

orbtensor 6 H

-1.782	-4.442	0.489
-4.442	-15.533	1.658
0.489	1.658	-0.573
28.014	4.152	-0.754
4.152	40.865	-2.555
-0.754	-2.555	25.479

orbtensor 7 C

-207.138	-15.410	4.567
-15.410	-254.837	15.467
4.567	15.467	-64.736
258.359	-2.453	-0.867
-2.453	250.766	-2.934
-0.867	-2.934	232.468

orbtensor 8 H

-11.608	7.635	-1.425
7.635	-5.706	0.977
-1.425	0.977	-0.573
37.197	-7.135	2.196
-7.135	31.681	-1.506
2.196	-1.506	25.479

orbtensor 9 C

-241.216	26.483	-13.292
26.483	-220.742	9.116
-13.292	9.116	-64.735
252.932	4.216	2.522
4.216	256.192	-1.730
2.522	-1.730	232.469

orbtensor 10 H

-10.757	-7.912	-1.370
-7.912	-6.557	-1.053
-1.370	-1.053	-0.573

36.401	7.394	2.111
7.394	32.477	1.624
2.111	1.624	25.479

orbtensor 11 C

-238.270	-27.444	-12.775
-27.444	-223.705	-9.830
-12.775	-9.830	-64.736
253.402	-4.369	2.423
-4.369	255.722	1.866
2.423	1.866	232.469

orbtensor 12 H

-1.780	-4.440	-0.489
-4.440	-15.534	-1.659
-0.489	-1.659	-0.573
28.012	4.149	0.753
4.149	40.866	2.556
0.753	2.556	25.480

orbtensor 13 C

-207.128	-15.401	-4.548
-15.401	-254.834	-15.486
-4.548	-15.486	-64.739
258.359	-2.452	0.861
-2.452	250.764	2.937
0.861	2.937	232.470

orbtensor 14 H

-11.611	7.634	1.427
7.634	-5.703	-0.978
1.427	-0.978	-0.574
37.200	-7.134	-2.199
-7.134	31.678	1.507
-2.199	1.507	25.480

orbtensor 15 C

-241.240	26.481	13.323
26.481	-220.745	-9.136
13.323	-9.136	-64.741
252.932	4.215	-2.526
4.215	256.194	1.731
-2.526	1.731	232.468

orbtensor 16 H

-10.755	-7.913	1.370
-7.913	-6.560	1.054
1.370	1.054	-0.573
36.400	7.395	-2.111
7.395	32.479	-1.624
-2.111	-1.624	25.479

orbtensor 17 C

-238.275	-27.449	12.796
-27.449	-223.725	9.820
12.796	9.820	-64.737
253.406	-4.368	-2.428
-4.368	255.722	-1.862
-2.428	-1.862	232.468

orbtensor 18 H

-2.309	5.169	-0.578
5.169	-15.006	1.626
-0.578	1.626	-0.573
28.507	-4.830	0.891
-4.830	40.372	-2.507
0.891	-2.507	25.479

```

orbtensor 19 C
-208.972   17.928   -5.388
17.928 -253.015   15.172
-5.388   15.172 -64.733
258.068   2.854   1.021
2.854  251.059  -2.881
1.021   -2.881  232.468

```

```

orbtensor 20 C
-259.330   -1.559  -16.100
-1.559 -202.630   -0.458
-16.100   -0.458 -64.733
250.048   -0.249   3.056
-0.249  259.075   0.087
3.056   0.087  232.469

```

```

orbtensor 21 H
-16.831   -0.450   -1.726
-0.450   -0.484   -0.048
-1.726   -0.048   -0.573
42.078   0.420   2.661
0.420  26.801   0.073
2.661   0.073  25.479

```

```

gtensor (ppt)
-0.149   0.000   0.000
0.000  -0.149   0.000
0.000   0.000  -0.168
-1.042   0.000   0.000
0.000  -1.042   0.000
0.000   0.000  -0.088

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-149.4913	1081.50200	142113.58815	-0.86103	142112.72712	143194.22912
2	H	-0.0750	25.48933	17.71047	-0.03460	17.67586	43.16520
3	C	1.6233	71.62067	-1524.16978	-0.34325	-1524.51303	-1452.89236
4	H	-0.0760	25.48967	17.94661	-0.03460	17.91200	43.40167
5	C	1.6237	71.62133	-1524.48275	-0.34335	-1524.82610	-1453.20476
6	H	-0.0740	25.49000	17.47433	-0.03460	17.43972	42.92972
7	C	1.6223	71.62733	-1523.23086	-0.34325	-1523.57411	-1451.94678
8	H	-0.0737	25.49000	17.39561	-0.03463	17.36099	42.85099
9	C	1.6210	71.63333	-1521.97898	-0.34315	-1522.32213	-1450.68880
10	H	-0.0740	25.49000	17.47433	-0.03460	17.43972	42.92972
11	C	1.6213	71.62733	-1522.29195	-0.34310	-1522.63505	-1451.00772
12	H	-0.0737	25.49033	17.39561	-0.03463	17.36099	42.85132
13	C	1.6217	71.63067	-1522.60492	-0.34320	-1522.94812	-1451.31746
14	H	-0.0753	25.49000	17.78918	-0.03465	17.75453	43.24453
15	C	1.6227	71.62267	-1523.54384	-0.34335	-1523.88718	-1452.26452
16	H	-0.0753	25.49000	17.78918	-0.03458	17.75460	43.24460
17	C	1.6237	71.61967	-1524.48275	-0.34335	-1524.82610	-1453.20643
18	H	-0.0743	25.49000	17.55304	-0.03458	17.51846	43.00846
19	C	1.6223	71.62500	-1523.23086	-0.34310	-1523.57397	-1451.94897
20	C	1.6213	71.63300	-1522.29195	-0.34310	-1522.63505	-1451.00205
21	H	-0.0737	25.49000	17.39561	-0.03463	17.36099	42.85099
13C Average		1.6223	71.62610	-1523.23086	-0.34322	-1523.57408	-1451.94798
1H Average		-0.0745	25.48993	17.59240	-0.03461	17.55779	43.04772

6MnCp2-STO-BHLYP-ORCA
Temperature: 390
Spin: 2.5

atensor 1 Mn
-148.584 0.000 0.001
0.000 -148.583 0.000
0.001 0.000 -139.835
-3.816 0.000 0.000
0.000 -3.816 0.000
0.000 0.000 -3.840

atensor 2 H
-2.322 -1.445 -1.237
-1.445 1.231 3.481
-1.237 3.481 0.866
0.001 0.001 0.000
0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 3 C
0.112 -0.275 -0.631
-0.275 0.787 1.776
-0.631 1.776 3.971
-0.001 -0.001 0.000
-0.001 0.001 0.000
0.001 -0.002 0.000

atensor 4 H
1.741 0.125 -3.693
0.125 -2.833 -0.101
-3.693 -0.101 0.865
-0.002 0.000 0.001
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C
0.885 0.024 -1.884
0.024 0.015 -0.051
-1.884 -0.051 3.972
0.001 0.000 -0.001
0.000 -0.002 0.000
0.002 0.000 0.000

atensor 6 H
-2.468 1.243 -1.045
1.243 1.379 -3.544
-1.045 -3.544 0.867
0.001 -0.001 0.000
-0.001 -0.001 0.001
0.000 0.001 0.000

atensor 7 C
0.083 0.236 -0.534
0.236 0.815 -1.808
-0.534 -1.808 3.970
-0.002 0.001 0.000
0.001 0.001 0.000
0.001 0.002 0.000

atensor 8 H
0.282 -2.136 3.048
-2.136 -1.370 -2.089
3.048 -2.089 0.868
-0.001 0.001 -0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 9 C
0.605 -0.406 1.555
-0.406 0.291 -1.066
1.555 -1.066 3.968
0.000 -0.002 0.000
-0.002 -0.001 0.000
-0.002 0.001 0.000

atensor 10 H
0.043 2.214 2.928
2.214 -1.132 2.253
2.928 2.253 0.867
0.000 -0.001 -0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 11 C
0.560 0.421 1.494
0.421 0.337 1.150
1.494 1.150 3.968
0.000 0.002 0.000
0.002 -0.001 0.000
-0.002 -0.001 0.000

atensor 12 H
-2.468 1.242 1.045
1.242 1.379 3.544
1.045 3.544 0.868
0.001 -0.001 0.000
-0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 13 C
0.083 0.236 0.533
0.236 0.814 1.808
0.533 1.808 3.969
-0.002 0.001 0.000
0.001 0.001 0.000
-0.001 -0.002 0.000

atensor 14 H
0.281 -2.135 -3.048
-2.135 -1.373 2.088
-3.048 2.088 0.867
-0.001 0.001 0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 15 C
0.606 -0.406 -1.555
-0.406 0.292 1.065
-1.555 1.065 3.971
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.002 -0.001 0.000

atensor 16 H
0.041 2.214 -2.927
2.214 -1.132 -2.253
-2.927 -2.253 0.865
0.000 -0.001 0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 17 C
0.561 0.421 -1.494

0.421 0.339 -1.150
-1.494 -1.150 3.972
0.000 0.002 0.000
0.002 -0.001 0.000
0.002 0.001 0.000

atensor 18 H
-2.321 -1.446 1.238
-1.446 1.232 -3.481
1.238 -3.481 0.866
0.001 0.001 0.000
0.001 -0.001 0.001
0.000 0.001 0.000

atensor 19 C
0.111 -0.275 0.631
-0.275 0.787 -1.777
0.631 -1.777 3.969
-0.001 -0.001 0.000
-0.001 0.001 0.000
-0.001 0.002 0.000

atensor 20 C
0.883 0.024 1.885
0.024 0.014 0.051
1.885 0.051 3.968
0.001 0.000 0.000
0.000 -0.002 0.000
-0.002 0.000 0.000

atensor 21 H
1.743 0.125 3.694
0.125 -2.831 0.101
3.694 0.101 0.868
-0.002 0.000 -0.001
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1234.995 -0.006 0.177
-0.006 -1235.004 -0.067
0.177 -0.067 -61.163
1922.996 0.000 0.001
0.000 1922.996 0.000
0.001 0.000 1929.676

orbtensor 2 H
-2.308 5.167 0.579
5.167 -15.008 -1.629
0.579 -1.629 -0.573
28.505 -4.828 -0.892
-4.828 40.373 2.510
-0.892 2.510 25.479

orbtensor 3 C
-208.972 17.922 5.407
17.922 -253.023 -15.197
5.407 -15.197 -64.738
258.069 2.852 -1.027
2.852 251.058 2.882
-1.027 2.882 232.468

orbtensor 4 H
-16.832 -0.448 1.728
-0.448 -0.483 0.047
1.728 0.047 -0.574
42.078 0.418 -2.663

0.418	26.801	-0.073
-2.663	-0.073	25.479

orbtensor 5 C

-259.350	-1.552	16.129
-1.552	-202.643	0.441
16.129	0.441	-64.738
250.051	-0.247	-3.059
-0.247	259.076	-0.084
-3.059	-0.084	232.468

orbtensor 6 H

-1.782	-4.442	0.489
-4.442	-15.533	1.658
0.489	1.658	-0.573
28.014	4.152	-0.754
4.152	40.865	-2.555
-0.754	-2.555	25.479

orbtensor 7 C

-207.138	-15.410	4.567
-15.410	-254.837	15.467
4.567	15.467	-64.736
258.359	-2.453	-0.867
-2.453	250.766	-2.934
-0.867	-2.934	232.468

orbtensor 8 H

-11.608	7.635	-1.425
7.635	-5.706	0.977
-1.425	0.977	-0.573
37.197	-7.135	2.196
-7.135	31.681	-1.506
2.196	-1.506	25.479

orbtensor 9 C

-241.216	26.483	-13.292
26.483	-220.742	9.116
-13.292	9.116	-64.735
252.932	4.216	2.522
4.216	256.192	-1.730
2.522	-1.730	232.469

orbtensor 10 H

-10.757	-7.912	-1.370
-7.912	-6.557	-1.053
-1.370	-1.053	-0.573
36.401	7.394	2.111
7.394	32.477	1.624
2.111	1.624	25.479

orbtensor 11 C

-238.270	-27.444	-12.775
-27.444	-223.705	-9.830
-12.775	-9.830	-64.736
253.402	-4.369	2.423
-4.369	255.722	1.866
2.423	1.866	232.469

orbtensor 12 H

-1.780	-4.440	-0.489
-4.440	-15.534	-1.659
-0.489	-1.659	-0.573
28.012	4.149	0.753
4.149	40.866	2.556
0.753	2.556	25.480

orbtensor 13 C
-207.128 -15.401 -4.548
-15.401 -254.834 -15.486
-4.548 -15.486 -64.739
258.359 -2.452 0.861
-2.452 250.764 2.937
0.861 2.937 232.470

orbtensor 14 H
-11.611 7.634 1.427
7.634 -5.703 -0.978
1.427 -0.978 -0.574
37.200 -7.134 -2.199
-7.134 31.678 1.507
-2.199 1.507 25.480

orbtensor 15 C
-241.240 26.481 13.323
26.481 -220.745 -9.136
13.323 -9.136 -64.741
252.932 4.215 -2.526
4.215 256.194 1.731
-2.526 1.731 232.468

orbtensor 16 H
-10.755 -7.913 1.370
-7.913 -6.560 1.054
1.370 1.054 -0.573
36.400 7.395 -2.111
7.395 32.479 -1.624
-2.111 -1.624 25.479

orbtensor 17 C
-238.275 -27.449 12.796
-27.449 -223.725 9.820
12.796 9.820 -64.737
253.406 -4.368 -2.428
-4.368 255.722 -1.862
-2.428 -1.862 232.468

orbtensor 18 H
-2.309 5.169 -0.578
5.169 -15.006 1.626
-0.578 1.626 -0.573
28.507 -4.830 0.891
-4.830 40.372 -2.507
0.891 -2.507 25.479

orbtensor 19 C
-208.972 17.928 -5.388
17.928 -253.015 15.172
-5.388 15.172 -64.733
258.068 2.854 1.021
2.854 251.059 -2.881
1.021 -2.881 232.468

orbtensor 20 C
-259.330 -1.559 -16.100
-1.559 -202.630 -0.458
-16.100 -0.458 -64.733
250.048 -0.249 3.056
-0.249 259.075 0.087
3.056 0.087 232.469

orbtensor 21 H
-16.831 -0.450 -1.726
-0.450 -0.484 -0.048

```

-1.726   -0.048   -0.573
42.078   0.420    2.661
0.420    26.801    0.073
2.661    0.073    25.479

```

```

gtensor (ppt)
-0.149   0.000   0.000
0.000   -0.149   0.000
0.000   0.000  -0.168
-1.042   0.000   0.000
0.000  -1.042   0.000
0.000   0.000  -0.088

```

```

zfstensor (cm-1)
4.306852  0.576479  0.000306
0.576479 -1.000578 -0.000144
0.000306 -0.000144 -0.804675

```

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-149.4913	1081.50200	142094.83252	-53.49774	142041.33478	143122.83678
2	H	-0.0750	25.48933	17.70813	-12.32740	5.38073	30.87006
3	C	1.6233	71.62067	-1523.96862	-29.04336	-1553.01199	-1481.39132
4	H	-0.0760	25.48967	17.94424	9.11310	27.05734	52.54700
5	C	1.6237	71.62133	-1524.28155	-12.77852	-1537.06007	-1465.43874
6	H	-0.0740	25.49000	17.47202	-10.19924	7.27278	32.76278
7	C	1.6223	71.62733	-1523.02983	-27.44255	-1550.47239	-1478.84506
8	H	-0.0737	25.49000	17.39332	-0.38695	17.00637	42.49637
9	C	1.6210	71.63333	-1521.77811	-19.97856	-1541.75667	-1470.12334
10	H	-0.0740	25.49000	17.47202	3.05477	20.52679	46.01679
11	C	1.6213	71.62733	-1522.09104	-17.36311	-1539.45416	-1467.82682
12	H	-0.0737	25.49033	17.39332	-10.20261	7.19071	32.68104
13	C	1.6217	71.63067	-1522.40397	-27.43143	-1549.83541	-1478.20474
14	H	-0.0753	25.49000	17.78683	-0.38713	17.39971	42.88971
15	C	1.6227	71.62267	-1523.34276	-19.99995	-1543.34272	-1471.72005
16	H	-0.0753	25.49000	17.78683	3.04937	20.83620	46.32620
17	C	1.6237	71.61967	-1524.28155	-17.39208	-1541.67363	-1470.05397
18	H	-0.0743	25.49000	17.55072	-12.32362	5.22711	30.71711
19	C	1.6223	71.62500	-1523.02983	-29.03724	-1552.06708	-1480.44208
20	C	1.6213	71.63300	-1522.09104	-12.76476	-1534.85580	-1463.22280
21	H	-0.0737	25.49000	17.39332	9.11567	26.50899	51.99899
13C Average		1.6223	71.62610	-1523.02983	-21.32316	-1544.35299	-1472.72689
1H Average		-0.0745	25.48993	17.59007	-2.14940	15.44067	40.93060

```

=====
6MnCp2-STO-BP-No-ZFS
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-56.877 0.000 -0.003
0.000 -56.876 0.000
-0.003 0.000 -59.915
-3.954 0.000 0.000
0.000 -3.954 0.000
0.000 0.000 -5.056

```

```

atensor 2 H
-2.328 -1.477 -1.181
-1.477 1.303 3.323

```

-1.181 3.323 0.886
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C
-0.401 -0.237 -0.619
-0.237 0.181 1.741
-0.619 1.741 4.053
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H
1.825 0.128 -3.525
0.128 -2.850 -0.096
-3.525 -0.096 0.886
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.265 0.020 -1.847
0.020 -0.485 -0.050
-1.847 -0.050 4.055
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.476 1.270 -0.998
1.270 1.456 -3.383
-0.998 -3.383 0.888
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.426 0.204 -0.523
0.204 0.205 -1.772
-0.523 -1.772 4.052
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.334 -2.183 2.909
-2.183 -1.354 -1.994
2.909 -1.994 0.889
0.001 -0.002 0.003
-0.002 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.024 -0.350 1.524
-0.350 -0.247 -1.045
1.524 -1.045 4.050
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.090 2.262 2.796
2.262 -1.111 2.151
2.796 2.151 0.888
0.001 0.002 0.002
0.002 0.000 0.002

0.000 0.000 0.000

atensor 11 C

-0.015 0.363 1.465
0.363 -0.207 1.127
1.465 1.127 4.051
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H

-2.476 1.270 0.997
1.270 1.456 3.383
0.997 3.383 0.890
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C

-0.426 0.204 0.522
0.204 0.204 1.772
0.522 1.772 4.051
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H

0.332 -2.182 -2.909
-2.182 -1.357 1.993
-2.909 1.993 0.887
0.001 -0.002 -0.003
-0.002 0.000 0.002
0.000 0.000 0.000

atensor 15 C

0.025 -0.350 -1.524
-0.350 -0.246 1.044
-1.524 1.044 4.054
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H

0.087 2.263 -2.794
2.263 -1.112 -2.151
-2.794 -2.151 0.885
0.001 0.002 -0.002
0.002 0.000 -0.002
0.000 0.000 0.000

atensor 17 C

-0.014 0.363 -1.464
0.363 -0.205 -1.127
-1.464 -1.127 4.055
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H

-2.326 -1.478 1.181
-1.478 1.305 -3.323
1.181 -3.323 0.886
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C

-0.402 -0.237 0.619
-0.237 0.181 -1.742
0.619 -1.742 4.052
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.264 0.020 1.847
0.020 -0.486 0.050
1.847 0.050 4.049
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.828 0.128 3.526
0.128 -2.847 0.096
3.526 0.096 0.889
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2972.697 -0.024 0.286
-0.024 -2972.766 -0.163
0.286 -0.163 -162.710
1936.724 0.000 0.002
0.000 1936.724 0.000
0.002 0.000 1934.404

orbtensor 2 H
-0.260 5.232 1.245
5.232 -13.119 -3.504
1.245 -3.504 -0.740
26.547 -4.283 -1.373
-4.283 37.074 3.863
-1.373 3.863 25.671

orbtensor 3 C
-179.324 22.577 8.225
22.577 -234.811 -23.130
8.225 -23.130 -62.363
228.901 -4.314 -3.778
-4.314 239.504 10.626
-3.778 10.626 225.041

orbtensor 4 H
-14.967 -0.453 3.718
-0.453 1.587 0.102
3.718 0.102 -0.739
38.586 0.371 -4.098
0.371 25.035 -0.112
-4.098 -0.112 25.670

orbtensor 5 C
-242.787 -1.954 24.541
-1.954 -171.361 0.671
24.541 0.671 -62.365
241.030 0.373 -11.272
0.373 227.382 -0.308
-11.272 -0.308 225.044

orbtensor 6 H
0.273 -4.498 1.052
-4.498 -13.651 3.568
1.052 3.568 -0.740

26.111	3.682	-1.160
3.682	37.509	-3.933
-1.160	-3.933	25.671

orbtensor 7 C

-177.019	-19.411	6.950
-19.411	-237.095	23.545
6.950	23.545	-62.362
228.459	3.710	-3.193
3.710	239.941	-10.818
-3.193	-10.818	225.041

orbtensor 8 H

-9.676	7.730	-3.067
7.730	-3.700	2.102
-3.067	2.102	-0.739
34.256	-6.329	3.381
-6.329	29.363	-2.318
3.381	-2.318	25.671

orbtensor 9 C

-219.940	33.353	-20.237
33.353	-194.156	13.876
-20.237	13.876	-62.364
236.663	-6.374	9.299
-6.374	231.735	-6.376
9.299	-6.376	225.046

orbtensor 10 H

-8.814	-8.011	-2.948
-8.011	-4.563	-2.268
-2.948	-2.268	-0.739
33.550	6.558	3.249
6.558	30.069	2.500
3.249	2.500	25.671

orbtensor 11 C

-216.223	-34.568	-19.450
-34.568	-197.881	-14.967
-19.450	-14.967	-62.361
235.950	6.607	8.939
6.607	232.445	6.878
8.939	6.878	225.041

orbtensor 12 H

0.274	-4.496	-1.052
-4.496	-13.651	-3.569
-1.052	-3.569	-0.740
26.109	3.680	1.159
3.680	37.510	3.934
1.159	3.934	25.672

orbtensor 13 C

-177.006	-19.396	-6.932
-19.396	-237.091	-23.563
-6.932	-23.563	-62.365
228.457	3.707	3.187
3.707	239.939	10.820
3.187	10.820	225.045

orbtensor 14 H

-9.680	7.730	3.069
7.730	-3.698	-2.103
3.069	-2.103	-0.740
34.259	-6.328	-3.383
-6.328	29.361	2.318
-3.383	2.318	25.671

orbtensor 15 C
-219.977 33.351 20.265
33.351 -194.161 -13.892
20.265 -13.892 -62.371
236.671 -6.372 -9.304
-6.372 231.737 6.374
-9.304 6.374 225.046

orbtensor 16 H
-8.814 -8.013 2.947
-8.013 -4.567 2.268
2.947 2.268 -0.739
33.549 6.559 -3.249
6.559 30.072 -2.500
-3.249 -2.500 25.670

orbtensor 17 C
-216.237 -34.576 19.464
-34.576 -197.910 14.958
19.464 14.958 -62.362
235.955 6.608 -8.938
6.608 232.455 -6.876
-8.938 -6.876 225.040

orbtensor 18 H
-0.261 5.233 -1.245
5.233 -13.118 3.502
-1.245 3.502 -0.738
26.548 -4.284 1.372
-4.284 37.073 -3.861
1.372 -3.861 25.670

orbtensor 19 C
-179.321 22.581 -8.210
22.581 -234.801 23.108
-8.210 23.108 -62.356
228.900 -4.316 3.776
-4.316 239.503 -10.625
3.776 -10.625 225.039

orbtensor 20 C
-242.754 -1.963 -24.517
-1.963 -171.343 -0.686
-24.517 -0.686 -62.361
241.024 0.374 11.270
0.374 227.375 0.310
11.270 0.310 225.045

orbtensor 21 H
-14.964 -0.455 -3.716
-0.455 1.587 -0.102
-3.716 -0.102 -0.738
38.585 0.373 4.097
0.373 25.034 0.113
4.097 0.113 25.670

gtensor (ppt)
-0.120 0.000 0.000
0.000 -0.120 0.000
0.000 0.000 -0.159
1.384 0.000 0.000
0.000 1.384 0.000
0.000 0.000 -0.133

averaging
C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-62.2107	-100.10700	59188.43267	-0.68003	59187.75264	59087.64564
2	H	-0.0460	25.05767	10.87124	0.05703	10.92827	35.98594
3	C	1.2813	72.31600	-1204.03790	0.67415	-1203.36375	-1131.04775
4	H	-0.0460	25.05733	10.87124	0.05703	10.92827	35.98560
5	C	1.2820	72.31433	-1204.66435	0.67447	-1203.98988	-1131.67555
6	H	-0.0437	25.05767	10.31980	0.05701	10.37681	35.43448
7	C	1.2807	72.32167	-1203.41145	0.67407	-1202.73739	-1130.41572
8	H	-0.0433	25.05833	10.24102	0.05705	10.29807	35.35641
9	C	1.2793	72.32800	-1202.15855	0.67391	-1201.48465	-1129.15665
10	H	-0.0440	25.05800	10.39857	0.05703	10.45561	35.51361
11	C	1.2800	72.32367	-1202.78500	0.67399	-1202.11102	-1129.78735
12	H	-0.0430	25.05800	10.16224	0.05709	10.21934	35.27734
13	C	1.2800	72.32633	-1202.78500	0.67399	-1202.11102	-1129.78468
14	H	-0.0457	25.05767	10.79246	0.05707	10.84953	35.90720
15	C	1.2813	72.31500	-1204.03790	0.67439	-1203.36351	-1131.04851
16	H	-0.0463	25.05700	10.95001	0.05699	11.00701	36.06401
17	C	1.2823	72.31367	-1204.97758	0.67439	-1204.30319	-1131.98952
18	H	-0.0447	25.05800	10.55613	0.05695	10.61308	35.67108
19	C	1.2807	72.32133	-1203.41145	0.67407	-1202.73739	-1130.41605
20	C	1.2793	72.32867	-1202.15855	0.67366	-1201.48489	-1129.15622
21	H	-0.0430	25.05800	10.16224	0.05703	10.21928	35.27728
C Average		1.2807	72.32087	-1203.44278	0.67411	-1202.76867	-1130.44780
H Average		-0.0446	25.05777	10.53250	0.05703	10.58953	35.64729

6MnCp2-STO-BP-Neese

Temperature: 390

Spin: 2.5

atensor 1 Mn

-56.877 0.000 -0.003
0.000 -56.876 0.000
-0.003 0.000 -59.915
-3.954 0.000 0.000
0.000 -3.954 0.000
0.000 0.000 -5.056

atensor 2 H

-2.328 -1.477 -1.181
-1.477 1.303 3.323
-1.181 3.323 0.886
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C

-0.401 -0.237 -0.619
-0.237 0.181 1.741
-0.619 1.741 4.053
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H

1.825 0.128 -3.525
0.128 -2.850 -0.096
-3.525 -0.096 0.886
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.265 0.020 -1.847
0.020 -0.485 -0.050
-1.847 -0.050 4.055
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.476 1.270 -0.998
1.270 1.456 -3.383
-0.998 -3.383 0.888
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.426 0.204 -0.523
0.204 0.205 -1.772
-0.523 -1.772 4.052
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.334 -2.183 2.909
-2.183 -1.354 -1.994
2.909 -1.994 0.889
0.001 -0.002 0.003
-0.002 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.024 -0.350 1.524
-0.350 -0.247 -1.045
1.524 -1.045 4.050
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.090 2.262 2.796
2.262 -1.111 2.151
2.796 2.151 0.888
0.001 0.002 0.002
0.002 0.000 0.002
0.000 0.000 0.000

atensor 11 C
-0.015 0.363 1.465
0.363 -0.207 1.127
1.465 1.127 4.051
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.476 1.270 0.997
1.270 1.456 3.383
0.997 3.383 0.890
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.426 0.204 0.522

0.204 0.204 1.772
0.522 1.772 4.051
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.332 -2.182 -2.909
-2.182 -1.357 1.993
-2.909 1.993 0.887
0.001 -0.002 -0.003
-0.002 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.025 -0.350 -1.524
-0.350 -0.246 1.044
-1.524 1.044 4.054
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.087 2.263 -2.794
2.263 -1.112 -2.151
-2.794 -2.151 0.885
0.001 0.002 -0.002
0.002 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
-0.014 0.363 -1.464
0.363 -0.205 -1.127
-1.464 -1.127 4.055
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.326 -1.478 1.181
-1.478 1.305 -3.323
1.181 -3.323 0.886
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.402 -0.237 0.619
-0.237 0.181 -1.742
0.619 -1.742 4.052
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.264 0.020 1.847
0.020 -0.486 0.050
1.847 0.050 4.049
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.828 0.128 3.526
0.128 -2.847 0.096
3.526 0.096 0.889
0.002 0.000 0.003

0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2972.697 -0.024 0.286
-0.024 -2972.766 -0.163
0.286 -0.163 -162.710
1936.724 0.000 0.002
0.000 1936.724 0.000
0.002 0.000 1934.404

orbtensor 2 H
-0.260 5.232 1.245
5.232 -13.119 -3.504
1.245 -3.504 -0.740
26.547 -4.283 -1.373
-4.283 37.074 3.863
-1.373 3.863 25.671

orbtensor 3 C
-179.324 22.577 8.225
22.577 -234.811 -23.130
8.225 -23.130 -62.363
228.901 -4.314 -3.778
-4.314 239.504 10.626
-3.778 10.626 225.041

orbtensor 4 H
-14.967 -0.453 3.718
-0.453 1.587 0.102
3.718 0.102 -0.739
38.586 0.371 -4.098
0.371 25.035 -0.112
-4.098 -0.112 25.670

orbtensor 5 C
-242.787 -1.954 24.541
-1.954 -171.361 0.671
24.541 0.671 -62.365
241.030 0.373 -11.272
0.373 227.382 -0.308
-11.272 -0.308 225.044

orbtensor 6 H
0.273 -4.498 1.052
-4.498 -13.651 3.568
1.052 3.568 -0.740
26.111 3.682 -1.160
3.682 37.509 -3.933
-1.160 -3.933 25.671

orbtensor 7 C
-177.019 -19.411 6.950
-19.411 -237.095 23.545
6.950 23.545 -62.362
228.459 3.710 -3.193
3.710 239.941 -10.818
-3.193 -10.818 225.041

orbtensor 8 H
-9.676 7.730 -3.067
7.730 -3.700 2.102
-3.067 2.102 -0.739
34.256 -6.329 3.381
-6.329 29.363 -2.318
3.381 -2.318 25.671

orbtensor 9 C
-219.940 33.353 -20.237
33.353 -194.156 13.876
-20.237 13.876 -62.364
236.663 -6.374 9.299
-6.374 231.735 -6.376
9.299 -6.376 225.046

orbtensor 10 H
-8.814 -8.011 -2.948
-8.011 -4.563 -2.268
-2.948 -2.268 -0.739
33.550 6.558 3.249
6.558 30.069 2.500
3.249 2.500 25.671

orbtensor 11 C
-216.223 -34.568 -19.450
-34.568 -197.881 -14.967
-19.450 -14.967 -62.361
235.950 6.607 8.939
6.607 232.445 6.878
8.939 6.878 225.041

orbtensor 12 H
0.274 -4.496 -1.052
-4.496 -13.651 -3.569
-1.052 -3.569 -0.740
26.109 3.680 1.159
3.680 37.510 3.934
1.159 3.934 25.672

orbtensor 13 C
-177.006 -19.396 -6.932
-19.396 -237.091 -23.563
-6.932 -23.563 -62.365
228.457 3.707 3.187
3.707 239.939 10.820
3.187 10.820 225.045

orbtensor 14 H
-9.680 7.730 3.069
7.730 -3.698 -2.103
3.069 -2.103 -0.740
34.259 -6.328 -3.383
-6.328 29.361 2.318
-3.383 2.318 25.671

orbtensor 15 C
-219.977 33.351 20.265
33.351 -194.161 -13.892
20.265 -13.892 -62.371
236.671 -6.372 -9.304
-6.372 231.737 6.374
-9.304 6.374 225.046

orbtensor 16 H
-8.814 -8.013 2.947
-8.013 -4.567 2.268
2.947 2.268 -0.739
33.549 6.559 -3.249
6.559 30.072 -2.500
-3.249 -2.500 25.670

orbtensor 17 C
-216.237 -34.576 19.464
-34.576 -197.910 14.958

19.464 14.958 -62.362
 235.955 6.608 -8.938
 6.608 232.455 -6.876
 -8.938 -6.876 225.040

orbtensor 18 H
 -0.261 5.233 -1.245
 5.233 -13.118 3.502
 -1.245 3.502 -0.738
 26.548 -4.284 1.372
 -4.284 37.073 -3.861
 1.372 -3.861 25.670

orbtensor 19 C
 -179.321 22.581 -8.210
 22.581 -234.801 23.108
 -8.210 23.108 -62.356
 228.900 -4.316 3.776
 -4.316 239.503 -10.625
 3.776 -10.625 225.039

orbtensor 20 C
 -242.754 -1.963 -24.517
 -1.963 -171.343 -0.686
 -24.517 -0.686 -62.361
 241.024 0.374 11.270
 0.374 227.375 0.310
 11.270 0.310 225.045

orbtensor 21 H
 -14.964 -0.455 -3.716
 -0.455 1.587 -0.102
 -3.716 -0.102 -0.738
 38.585 0.373 4.097
 0.373 25.034 0.113
 4.097 0.113 25.670

gtensor (ppt)
 -0.120 0.000 0.000
 0.000 -0.120 0.000
 0.000 0.000 -0.159
 1.384 0.000 0.000
 0.000 1.384 0.000
 0.000 0.000 -0.133

zfstensor (cm-1)
 0.115722 -0.000026 0.000069
 -0.000026 0.115749 -0.000024
 0.000069 -0.000024 -0.231471

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-62.2107	-100.10700	59188.35621	2.91021	59191.26641	59091.15941
2	H	-0.0460	25.05767	10.87122	-0.24426	10.62696	35.68463
3	C	1.2813	72.31600	-1204.03635	-2.88560	-1206.92194	-1134.60594
4	H	-0.0460	25.05733	10.87122	-0.24459	10.62663	35.68396
5	C	1.2820	72.31433	-1204.66280	-2.88741	-1207.55021	-1135.23587
6	H	-0.0437	25.05767	10.31978	-0.24398	10.07580	35.13347
7	C	1.2807	72.32167	-1203.40990	-2.88466	-1206.29456	-1133.97289
8	H	-0.0433	25.05833	10.24101	-0.24362	9.99739	35.05572
9	C	1.2793	72.32800	-1202.15700	-2.88299	-1205.03999	-1132.71199

10	H	-0.0440	25.05800	10.39856	-0.24394	10.15462	35.21262
11	C	1.2800	72.32367	-1202.78345	-2.88388	-1205.66733	-1133.34367
12	H	-0.0430	25.05800	10.16223	-0.24437	9.91786	34.97586
13	C	1.2800	72.32633	-1202.78345	-2.88441	-1205.66786	-1133.34152
14	H	-0.0457	25.05767	10.79245	-0.24463	10.54781	35.60548
15	C	1.2813	72.31500	-1204.03635	-2.88700	-1206.92335	-1134.60835
16	H	-0.0463	25.05700	10.95000	-0.24429	10.70571	35.76271
17	C	1.2823	72.31367	-1204.97602	-2.88671	-1207.86274	-1135.54907
18	H	-0.0447	25.05800	10.55611	-0.24331	10.31280	35.37080
19	C	1.2807	72.32133	-1203.40990	-2.88400	-1206.29390	-1133.97256
20	C	1.2793	72.32867	-1202.15700	-2.88207	-1205.03907	-1132.71040
21	H	-0.0430	25.05800	10.16223	-0.24369	9.91854	34.97654
C Average		1.2807	72.32087	-1203.44122	-2.88487	-1206.32609	-1134.00523
H Average		-0.0446	25.05777	10.53248	-0.24407	10.28841	35.34618

=====

6MnCp2-STO-BP-ORCA

Temperature: 390

Spin: 2.5

atensor 1 Mn

-56.877 0.000 -0.003
0.000 -56.876 0.000
-0.003 0.000 -59.915
-3.954 0.000 0.000
0.000 -3.954 0.000
0.000 0.000 -5.056

atensor 2 H

-2.328 -1.477 -1.181
-1.477 1.303 3.323
-1.181 3.323 0.886
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C

-0.401 -0.237 -0.619
-0.237 0.181 1.741
-0.619 1.741 4.053
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H

1.825 0.128 -3.525
0.128 -2.850 -0.096
-3.525 -0.096 0.886
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C

0.265 0.020 -1.847
0.020 -0.485 -0.050
-1.847 -0.050 4.055
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H

-2.476 1.270 -0.998
1.270 1.456 -3.383
-0.998 -3.383 0.888
-0.001 0.001 -0.001
0.001 0.002 -0.003

0.000 0.000 0.000

atensor 7 C
-0.426 0.204 -0.523
0.204 0.205 -1.772
-0.523 -1.772 4.052
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.334 -2.183 2.909
-2.183 -1.354 -1.994
2.909 -1.994 0.889
0.001 -0.002 0.003
-0.002 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.024 -0.350 1.524
-0.350 -0.247 -1.045
1.524 -1.045 4.050
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.090 2.262 2.796
2.262 -1.111 2.151
2.796 2.151 0.888
0.001 0.002 0.002
0.002 0.000 0.002
0.000 0.000 0.000

atensor 11 C
-0.015 0.363 1.465
0.363 -0.207 1.127
1.465 1.127 4.051
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.476 1.270 0.997
1.270 1.456 3.383
0.997 3.383 0.890
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.426 0.204 0.522
0.204 0.204 1.772
0.522 1.772 4.051
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.332 -2.182 -2.909
-2.182 -1.357 1.993
-2.909 1.993 0.887
0.001 -0.002 -0.003
-0.002 0.000 0.002
0.000 0.000 0.000

atensor 15 C

0.025 -0.350 -1.524
-0.350 -0.246 1.044
-1.524 1.044 4.054
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.087 2.263 -2.794
2.263 -1.112 -2.151
-2.794 -2.151 0.885
0.001 0.002 -0.002
0.002 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
-0.014 0.363 -1.464
0.363 -0.205 -1.127
-1.464 -1.127 4.055
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.326 -1.478 1.181
-1.478 1.305 -3.323
1.181 -3.323 0.886
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.402 -0.237 0.619
-0.237 0.181 -1.742
0.619 -1.742 4.052
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.264 0.020 1.847
0.020 -0.486 0.050
1.847 0.050 4.049
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.828 0.128 3.526
0.128 -2.847 0.096
3.526 0.096 0.889
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2972.697 -0.024 0.286
-0.024 -2972.766 -0.163
0.286 -0.163 -162.710
1936.724 0.000 0.002
0.000 1936.724 0.000
0.002 0.000 1934.404

orbtensor 2 H
-0.260 5.232 1.245
5.232 -13.119 -3.504
1.245 -3.504 -0.740

26.547	-4.283	-1.373
-4.283	37.074	3.863
-1.373	3.863	25.671

orbtensor 3 C

-179.324	22.577	8.225
22.577	-234.811	-23.130
8.225	-23.130	-62.363
228.901	-4.314	-3.778
-4.314	239.504	10.626
-3.778	10.626	225.041

orbtensor 4 H

-14.967	-0.453	3.718
-0.453	1.587	0.102
3.718	0.102	-0.739
38.586	0.371	-4.098
0.371	25.035	-0.112
-4.098	-0.112	25.670

orbtensor 5 C

-242.787	-1.954	24.541
-1.954	-171.361	0.671
24.541	0.671	-62.365
241.030	0.373	-11.272
0.373	227.382	-0.308
-11.272	-0.308	225.044

orbtensor 6 H

0.273	-4.498	1.052
-4.498	-13.651	3.568
1.052	3.568	-0.740
26.111	3.682	-1.160
3.682	37.509	-3.933
-1.160	-3.933	25.671

orbtensor 7 C

-177.019	-19.411	6.950
-19.411	-237.095	23.545
6.950	23.545	-62.362
228.459	3.710	-3.193
3.710	239.941	-10.818
-3.193	-10.818	225.041

orbtensor 8 H

-9.676	7.730	-3.067
7.730	-3.700	2.102
-3.067	2.102	-0.739
34.256	-6.329	3.381
-6.329	29.363	-2.318
3.381	-2.318	25.671

orbtensor 9 C

-219.940	33.353	-20.237
33.353	-194.156	13.876
-20.237	13.876	-62.364
236.663	-6.374	9.299
-6.374	231.735	-6.376
9.299	-6.376	225.046

orbtensor 10 H

-8.814	-8.011	-2.948
-8.011	-4.563	-2.268
-2.948	-2.268	-0.739
33.550	6.558	3.249
6.558	30.069	2.500
3.249	2.500	25.671

orbtensor 11 C
-216.223 -34.568 -19.450
-34.568 -197.881 -14.967
-19.450 -14.967 -62.361
235.950 6.607 8.939
6.607 232.445 6.878
8.939 6.878 225.041

orbtensor 12 H
0.274 -4.496 -1.052
-4.496 -13.651 -3.569
-1.052 -3.569 -0.740
26.109 3.680 1.159
3.680 37.510 3.934
1.159 3.934 25.672

orbtensor 13 C
-177.006 -19.396 -6.932
-19.396 -237.091 -23.563
-6.932 -23.563 -62.365
228.457 3.707 3.187
3.707 239.939 10.820
3.187 10.820 225.045

orbtensor 14 H
-9.680 7.730 3.069
7.730 -3.698 -2.103
3.069 -2.103 -0.740
34.259 -6.328 -3.383
-6.328 29.361 2.318
-3.383 2.318 25.671

orbtensor 15 C
-219.977 33.351 20.265
33.351 -194.161 -13.892
20.265 -13.892 -62.371
236.671 -6.372 -9.304
-6.372 231.737 6.374
-9.304 6.374 225.046

orbtensor 16 H
-8.814 -8.013 2.947
-8.013 -4.567 2.268
2.947 2.268 -0.739
33.549 6.559 -3.249
6.559 30.072 -2.500
-3.249 -2.500 25.670

orbtensor 17 C
-216.237 -34.576 19.464
-34.576 -197.910 14.958
19.464 14.958 -62.362
235.955 6.608 -8.938
6.608 232.455 -6.876
-8.938 -6.876 225.040

orbtensor 18 H
-0.261 5.233 -1.245
5.233 -13.118 3.502
-1.245 3.502 -0.738
26.548 -4.284 1.372
-4.284 37.073 -3.861
1.372 -3.861 25.670

orbtensor 19 C
-179.321 22.581 -8.210

```

22.581 -234.801 23.108
-8.210 23.108 -62.356
228.900 -4.316 3.776
-4.316 239.503 -10.625
3.776 -10.625 225.039

```

```

orbtensor 20 C
-242.754 -1.963 -24.517
-1.963 -171.343 -0.686
-24.517 -0.686 -62.361
241.024 0.374 11.270
0.374 227.375 0.310
11.270 0.310 225.045

```

```

orbtensor 21 H
-14.964 -0.455 -3.716
-0.455 1.587 -0.102
-3.716 -0.102 -0.738
38.585 0.373 4.097
0.373 25.034 0.113
4.097 0.113 25.670

```

```

gtensor (ppt)
-0.120 0.000 0.000
0.000 -0.120 0.000
0.000 0.000 -0.159
1.384 0.000 0.000
0.000 1.384 0.000
0.000 0.000 -0.133

```

```

zfstensor (cm-1)
0.115722 -0.000026 0.000069
-0.000026 0.115749 -0.000024
0.000069 -0.000024 -0.231471

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-62.2107	-100.10700	59188.35621	2.91021	59191.26641	59091.15941
2	H	-0.0460	25.05767	10.87122	-0.24426	10.62696	35.68463
3	C	1.2813	72.31600	-1204.03635	-2.88560	-1206.92194	-1134.60594
4	H	-0.0460	25.05733	10.87122	-0.24459	10.62663	35.68396
5	C	1.2820	72.31433	-1204.66280	-2.88741	-1207.55021	-1135.23587
6	H	-0.0437	25.05767	10.31978	-0.24398	10.07580	35.13347
7	C	1.2807	72.32167	-1203.40990	-2.88466	-1206.29456	-1133.97289
8	H	-0.0433	25.05833	10.24101	-0.24362	9.99739	35.05572
9	C	1.2793	72.32800	-1202.15700	-2.88299	-1205.03999	-1132.71199
10	H	-0.0440	25.05800	10.39856	-0.24394	10.15462	35.21262
11	C	1.2800	72.32367	-1202.78345	-2.88388	-1205.66733	-1133.34367
12	H	-0.0430	25.05800	10.16223	-0.24437	9.91786	34.97586
13	C	1.2800	72.32633	-1202.78345	-2.88441	-1205.66786	-1133.34152
14	H	-0.0457	25.05767	10.79245	-0.24463	10.54781	35.60548
15	C	1.2813	72.31500	-1204.03635	-2.88700	-1206.92335	-1134.60835
16	H	-0.0463	25.05700	10.95000	-0.24429	10.70571	35.76271
17	C	1.2823	72.31367	-1204.97602	-2.88671	-1207.86274	-1135.54907
18	H	-0.0447	25.05800	10.55611	-0.24331	10.31280	35.37080
19	C	1.2807	72.32133	-1203.40990	-2.88400	-1206.29390	-1133.97256
20	C	1.2793	72.32867	-1202.15700	-2.88207	-1205.03907	-1132.71040
21	H	-0.0430	25.05800	10.16223	-0.24369	9.91854	34.97654
C Average		1.2807	72.32087	-1203.44122	-2.88487	-1206.32609	-1134.00523
H Average		-0.0446	25.05777	10.53248	-0.24407	10.28841	35.34618

=====
6MnCp2-STO-BP-Pederson

Temperature: 390

Spin: 2.5

atensor 1 Mn

-56.877 0.000 -0.003
0.000 -56.876 0.000
-0.003 0.000 -59.915
-3.954 0.000 0.000
0.000 -3.954 0.000
0.000 0.000 -5.056

atensor 2 H

-2.328 -1.477 -1.181
-1.477 1.303 3.323
-1.181 3.323 0.886
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C

-0.401 -0.237 -0.619
-0.237 0.181 1.741
-0.619 1.741 4.053
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H

1.825 0.128 -3.525
0.128 -2.850 -0.096
-3.525 -0.096 0.886
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C

0.265 0.020 -1.847
0.020 -0.485 -0.050
-1.847 -0.050 4.055
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H

-2.476 1.270 -0.998
1.270 1.456 -3.383
-0.998 -3.383 0.888
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C

-0.426 0.204 -0.523
0.204 0.205 -1.772
-0.523 -1.772 4.052
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H

0.334 -2.183 2.909
-2.183 -1.354 -1.994
2.909 -1.994 0.889
0.001 -0.002 0.003

-0.002 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.024 -0.350 1.524
-0.350 -0.247 -1.045
1.524 -1.045 4.050
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.090 2.262 2.796
2.262 -1.111 2.151
2.796 2.151 0.888
0.001 0.002 0.002
0.002 0.000 0.002
0.000 0.000 0.000

atensor 11 C
-0.015 0.363 1.465
0.363 -0.207 1.127
1.465 1.127 4.051
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.476 1.270 0.997
1.270 1.456 3.383
0.997 3.383 0.890
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.426 0.204 0.522
0.204 0.204 1.772
0.522 1.772 4.051
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.332 -2.182 -2.909
-2.182 -1.357 1.993
-2.909 1.993 0.887
0.001 -0.002 -0.003
-0.002 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.025 -0.350 -1.524
-0.350 -0.246 1.044
-1.524 1.044 4.054
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.087 2.263 -2.794
2.263 -1.112 -2.151
-2.794 -2.151 0.885
0.001 0.002 -0.002
0.002 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
-0.014 0.363 -1.464
0.363 -0.205 -1.127
-1.464 -1.127 4.055
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.326 -1.478 1.181
-1.478 1.305 -3.323
1.181 -3.323 0.886
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.402 -0.237 0.619
-0.237 0.181 -1.742
0.619 -1.742 4.052
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.264 0.020 1.847
0.020 -0.486 0.050
1.847 0.050 4.049
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.828 0.128 3.526
0.128 -2.847 0.096
3.526 0.096 0.889
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2972.697 -0.024 0.286
-0.024 -2972.766 -0.163
0.286 -0.163 -162.710
1936.724 0.000 0.002
0.000 1936.724 0.000
0.002 0.000 1934.404

orbtensor 2 H
-0.260 5.232 1.245
5.232 -13.119 -3.504
1.245 -3.504 -0.740
26.547 -4.283 -1.373
-4.283 37.074 3.863
-1.373 3.863 25.671

orbtensor 3 C
-179.324 22.577 8.225
22.577 -234.811 -23.130
8.225 -23.130 -62.363
228.901 -4.314 -3.778
-4.314 239.504 10.626
-3.778 10.626 225.041

orbtensor 4 H
-14.967 -0.453 3.718
-0.453 1.587 0.102

3.718	0.102	-0.739
38.586	0.371	-4.098
0.371	25.035	-0.112
-4.098	-0.112	25.670

orbtensor 5 C

-242.787	-1.954	24.541
-1.954	-171.361	0.671
24.541	0.671	-62.365
241.030	0.373	-11.272
0.373	227.382	-0.308
-11.272	-0.308	225.044

orbtensor 6 H

0.273	-4.498	1.052
-4.498	-13.651	3.568
1.052	3.568	-0.740
26.111	3.682	-1.160
3.682	37.509	-3.933
-1.160	-3.933	25.671

orbtensor 7 C

-177.019	-19.411	6.950
-19.411	-237.095	23.545
6.950	23.545	-62.362
228.459	3.710	-3.193
3.710	239.941	-10.818
-3.193	-10.818	225.041

orbtensor 8 H

-9.676	7.730	-3.067
7.730	-3.700	2.102
-3.067	2.102	-0.739
34.256	-6.329	3.381
-6.329	29.363	-2.318
3.381	-2.318	25.671

orbtensor 9 C

-219.940	33.353	-20.237
33.353	-194.156	13.876
-20.237	13.876	-62.364
236.663	-6.374	9.299
-6.374	231.735	-6.376
9.299	-6.376	225.046

orbtensor 10 H

-8.814	-8.011	-2.948
-8.011	-4.563	-2.268
-2.948	-2.268	-0.739
33.550	6.558	3.249
6.558	30.069	2.500
3.249	2.500	25.671

orbtensor 11 C

-216.223	-34.568	-19.450
-34.568	-197.881	-14.967
-19.450	-14.967	-62.361
235.950	6.607	8.939
6.607	232.445	6.878
8.939	6.878	225.041

orbtensor 12 H

0.274	-4.496	-1.052
-4.496	-13.651	-3.569
-1.052	-3.569	-0.740
26.109	3.680	1.159
3.680	37.510	3.934

1.159	3.934	25.672
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orbtensor 13 C

-177.006	-19.396	-6.932
-19.396	-237.091	-23.563
-6.932	-23.563	-62.365
228.457	3.707	3.187
3.707	239.939	10.820
3.187	10.820	225.045

orbtensor 14 H

-9.680	7.730	3.069
7.730	-3.698	-2.103
3.069	-2.103	-0.740
34.259	-6.328	-3.383
-6.328	29.361	2.318
-3.383	2.318	25.671

orbtensor 15 C

-219.977	33.351	20.265
33.351	-194.161	-13.892
20.265	-13.892	-62.371
236.671	-6.372	-9.304
-6.372	231.737	6.374
-9.304	6.374	225.046

orbtensor 16 H

-8.814	-8.013	2.947
-8.013	-4.567	2.268
2.947	2.268	-0.739
33.549	6.559	-3.249
6.559	30.072	-2.500
-3.249	-2.500	25.670

orbtensor 17 C

-216.237	-34.576	19.464
-34.576	-197.910	14.958
19.464	14.958	-62.362
235.955	6.608	-8.938
6.608	232.455	-6.876
-8.938	-6.876	225.040

orbtensor 18 H

-0.261	5.233	-1.245
5.233	-13.118	3.502
-1.245	3.502	-0.738
26.548	-4.284	1.372
-4.284	37.073	-3.861
1.372	-3.861	25.670

orbtensor 19 C

-179.321	22.581	-8.210
22.581	-234.801	23.108
-8.210	23.108	-62.356
228.900	-4.316	3.776
-4.316	239.503	-10.625
3.776	-10.625	225.039

orbtensor 20 C

-242.754	-1.963	-24.517
-1.963	-171.343	-0.686
-24.517	-0.686	-62.361
241.024	0.374	11.270
0.374	227.375	0.310
11.270	0.310	225.045

orbtensor 21 H

```

-14.964  -0.455  -3.716
-0.455   1.587  -0.102
-3.716  -0.102  -0.738
38.585   0.373   4.097
0.373   25.034   0.113
4.097   0.113   25.670

```

gtensor (ppt)

```

-0.120   0.000   0.000
 0.000  -0.120   0.000
 0.000   0.000  -0.159
1.384   0.000   0.000
0.000   1.384   0.000
0.000   0.000  -0.133

```

zfstensor (cm-1)

```

0.088117  -0.000020   0.000064
-0.000020   0.088140  -0.000018
0.000064  -0.000018  -0.176257

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-62.2107	-100.10700	59188.38073	2.05327	59190.43400	59090.32700
2	H	-0.0460	25.05767	10.87123	-0.17237	10.69886	35.75653
3	C	1.2813	72.31600	-1204.03685	-2.03599	-1206.07284	-1133.75684
4	H	-0.0460	25.05733	10.87123	-0.17268	10.69855	35.75588
5	C	1.2820	72.31433	-1204.66330	-2.03741	-1206.70070	-1134.38637
6	H	-0.0437	25.05767	10.31979	-0.17216	10.14763	35.20530
7	C	1.2807	72.32167	-1203.41040	-2.03529	-1205.44569	-1133.12402
8	H	-0.0433	25.05833	10.24101	-0.17179	10.06922	35.12755
9	C	1.2793	72.32800	-1202.15750	-2.03389	-1204.19138	-1131.86338
10	H	-0.0440	25.05800	10.39856	-0.17204	10.22652	35.28452
11	C	1.2800	72.32367	-1202.78395	-2.03455	-1204.81850	-1132.49483
12	H	-0.0430	25.05800	10.16223	-0.17239	9.98984	35.04784
13	C	1.2800	72.32633	-1202.78395	-2.03503	-1204.81897	-1132.49264
14	H	-0.0457	25.05767	10.79245	-0.17268	10.61977	35.67744
15	C	1.2813	72.31500	-1204.03685	-2.03708	-1206.07393	-1133.75893
16	H	-0.0463	25.05700	10.95000	-0.17244	10.77756	35.83456
17	C	1.2823	72.31367	-1204.97652	-2.03686	-1207.01339	-1134.69972
18	H	-0.0447	25.05800	10.55612	-0.17161	10.38450	35.44250
19	C	1.2807	72.32133	-1203.41040	-2.03469	-1205.44509	-1133.12376
20	C	1.2793	72.32867	-1202.15750	-2.03322	-1204.19072	-1131.86205
21	H	-0.0430	25.05800	10.16223	-0.17184	9.99039	35.04839
C Average		1.2807	72.32087	-1203.44172	-2.03540	-1205.47712	-1133.15625
H Average		-0.0446	25.05777	10.53249	-0.17220	10.36028	35.41805

6MnCp2-STO-BP-Van-Wullen

Temperature: 390

Spin: 2.5

atensor 1 Mn

```

-56.877 0.000 -0.003
0.000 -56.876 0.000
-0.003 0.000 -59.915
-3.954 0.000 0.000
0.000 -3.954 0.000
0.000 0.000 -5.056

```

atensor 2 H

-2.328 -1.477 -1.181
-1.477 1.303 3.323
-1.181 3.323 0.886
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C
-0.401 -0.237 -0.619
-0.237 0.181 1.741
-0.619 1.741 4.053
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H
1.825 0.128 -3.525
0.128 -2.850 -0.096
-3.525 -0.096 0.886
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.265 0.020 -1.847
0.020 -0.485 -0.050
-1.847 -0.050 4.055
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.476 1.270 -0.998
1.270 1.456 -3.383
-0.998 -3.383 0.888
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.426 0.204 -0.523
0.204 0.205 -1.772
-0.523 -1.772 4.052
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.334 -2.183 2.909
-2.183 -1.354 -1.994
2.909 -1.994 0.889
0.001 -0.002 0.003
-0.002 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.024 -0.350 1.524
-0.350 -0.247 -1.045
1.524 -1.045 4.050
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.090 2.262 2.796
2.262 -1.111 2.151
2.796 2.151 0.888

0.001 0.002 0.002
0.002 0.000 0.002
0.000 0.000 0.000

atensor 11 C
-0.015 0.363 1.465
0.363 -0.207 1.127
1.465 1.127 4.051
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.476 1.270 0.997
1.270 1.456 3.383
0.997 3.383 0.890
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.426 0.204 0.522
0.204 0.204 1.772
0.522 1.772 4.051
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.332 -2.182 -2.909
-2.182 -1.357 1.993
-2.909 1.993 0.887
0.001 -0.002 -0.003
-0.002 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.025 -0.350 -1.524
-0.350 -0.246 1.044
-1.524 1.044 4.054
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.087 2.263 -2.794
2.263 -1.112 -2.151
-2.794 -2.151 0.885
0.001 0.002 -0.002
0.002 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
-0.014 0.363 -1.464
0.363 -0.205 -1.127
-1.464 -1.127 4.055
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.326 -1.478 1.181
-1.478 1.305 -3.323
1.181 -3.323 0.886
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.402 -0.237 0.619
-0.237 0.181 -1.742
0.619 -1.742 4.052
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.264 0.020 1.847
0.020 -0.486 0.050
1.847 0.050 4.049
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.828 0.128 3.526
0.128 -2.847 0.096
3.526 0.096 0.889
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2972.697 -0.024 0.286
-0.024 -2972.766 -0.163
0.286 -0.163 -162.710
1936.724 0.000 0.002
0.000 1936.724 0.000
0.002 0.000 1934.404

orbtensor 2 H
-0.260 5.232 1.245
5.232 -13.119 -3.504
1.245 -3.504 -0.740
26.547 -4.283 -1.373
-4.283 37.074 3.863
-1.373 3.863 25.671

orbtensor 3 C
-179.324 22.577 8.225
22.577 -234.811 -23.130
8.225 -23.130 -62.363
228.901 -4.314 -3.778
-4.314 239.504 10.626
-3.778 10.626 225.041

orbtensor 4 H
-14.967 -0.453 3.718
-0.453 1.587 0.102
3.718 0.102 -0.739
38.586 0.371 -4.098
0.371 25.035 -0.112
-4.098 -0.112 25.670

orbtensor 5 C
-242.787 -1.954 24.541
-1.954 -171.361 0.671
24.541 0.671 -62.365
241.030 0.373 -11.272
0.373 227.382 -0.308
-11.272 -0.308 225.044

orbtensor 6 H
0.273 -4.498 1.052

-4.498	-13.651	3.568
1.052	3.568	-0.740
26.111	3.682	-1.160
3.682	37.509	-3.933
-1.160	-3.933	25.671

orbtensor 7 C

-177.019	-19.411	6.950
-19.411	-237.095	23.545
6.950	23.545	-62.362
228.459	3.710	-3.193
3.710	239.941	-10.818
-3.193	-10.818	225.041

orbtensor 8 H

-9.676	7.730	-3.067
7.730	-3.700	2.102
-3.067	2.102	-0.739
34.256	-6.329	3.381
-6.329	29.363	-2.318
3.381	-2.318	25.671

orbtensor 9 C

-219.940	33.353	-20.237
33.353	-194.156	13.876
-20.237	13.876	-62.364
236.663	-6.374	9.299
-6.374	231.735	-6.376
9.299	-6.376	225.046

orbtensor 10 H

-8.814	-8.011	-2.948
-8.011	-4.563	-2.268
-2.948	-2.268	-0.739
33.550	6.558	3.249
6.558	30.069	2.500
3.249	2.500	25.671

orbtensor 11 C

-216.223	-34.568	-19.450
-34.568	-197.881	-14.967
-19.450	-14.967	-62.361
235.950	6.607	8.939
6.607	232.445	6.878
8.939	6.878	225.041

orbtensor 12 H

0.274	-4.496	-1.052
-4.496	-13.651	-3.569
-1.052	-3.569	-0.740
26.109	3.680	1.159
3.680	37.510	3.934
1.159	3.934	25.672

orbtensor 13 C

-177.006	-19.396	-6.932
-19.396	-237.091	-23.563
-6.932	-23.563	-62.365
228.457	3.707	3.187
3.707	239.939	10.820
3.187	10.820	225.045

orbtensor 14 H

-9.680	7.730	3.069
7.730	-3.698	-2.103
3.069	-2.103	-0.740
34.259	-6.328	-3.383

-6.328	29.361	2.318
-3.383	2.318	25.671
orbtensor 15 C		
-219.977	33.351	20.265
33.351	-194.161	-13.892
20.265	-13.892	-62.371
236.671	-6.372	-9.304
-6.372	231.737	6.374
-9.304	6.374	225.046
orbtensor 16 H		
-8.814	-8.013	2.947
-8.013	-4.567	2.268
2.947	2.268	-0.739
33.549	6.559	-3.249
6.559	30.072	-2.500
-3.249	-2.500	25.670
orbtensor 17 C		
-216.237	-34.576	19.464
-34.576	-197.910	14.958
19.464	14.958	-62.362
235.955	6.608	-8.938
6.608	232.455	-6.876
-8.938	-6.876	225.040
orbtensor 18 H		
-0.261	5.233	-1.245
5.233	-13.118	3.502
-1.245	3.502	-0.738
26.548	-4.284	1.372
-4.284	37.073	-3.861
1.372	-3.861	25.670
orbtensor 19 C		
-179.321	22.581	-8.210
22.581	-234.801	23.108
-8.210	23.108	-62.356
228.900	-4.316	3.776
-4.316	239.503	-10.625
3.776	-10.625	225.039
orbtensor 20 C		
-242.754	-1.963	-24.517
-1.963	-171.343	-0.686
-24.517	-0.686	-62.361
241.024	0.374	11.270
0.374	227.375	0.310
11.270	0.310	225.045
orbtensor 21 H		
-14.964	-0.455	-3.716
-0.455	1.587	-0.102
-3.716	-0.102	-0.738
38.585	0.373	4.097
0.373	25.034	0.113
4.097	0.113	25.670
gtensor (ppt)		
-0.120	0.000	0.000
0.000	-0.120	0.000
0.000	0.000	-0.159
1.384	0.000	0.000
0.000	1.384	0.000
0.000	0.000	-0.133

```

zfstensor (cm-1)
0.110146 -0.000025 0.000080
-0.000025 0.110174 -0.000022
0.000080 -0.000022 -0.220321

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-62.2107	-100.10700	59188.36148	2.73712	59191.09860	59090.99160
2	H	-0.0460	25.05767	10.87122	-0.22976	10.64147	35.69913
3	C	1.2813	72.31600	-1204.03646	-2.71404	-1206.75049	-1134.43449
4	H	-0.0460	25.05733	10.87122	-0.23015	10.64107	35.69841
5	C	1.2820	72.31433	-1204.66291	-2.71589	-1207.37880	-1135.06447
6	H	-0.0437	25.05767	10.31978	-0.22950	10.09029	35.14795
7	C	1.2807	72.32167	-1203.41001	-2.71316	-1206.12317	-1133.80150
8	H	-0.0433	25.05833	10.24101	-0.22905	10.01196	35.07029
9	C	1.2793	72.32800	-1202.15711	-2.71136	-1204.86846	-1132.54046
10	H	-0.0440	25.05800	10.39856	-0.22935	10.16921	35.22721
11	C	1.2800	72.32367	-1202.78356	-2.71220	-1205.49576	-1133.17209
12	H	-0.0430	25.05800	10.16223	-0.22981	9.93243	34.99043
13	C	1.2800	72.32633	-1202.78356	-2.71279	-1205.49635	-1133.17001
14	H	-0.0457	25.05767	10.79245	-0.23016	10.56229	35.61995
15	C	1.2813	72.31500	-1204.03646	-2.71546	-1206.75192	-1134.43692
16	H	-0.0463	25.05700	10.95000	-0.22985	10.72015	35.77715
17	C	1.2823	72.31367	-1204.97613	-2.71520	-1207.69133	-1135.37766
18	H	-0.0447	25.05800	10.55612	-0.22880	10.32731	35.38531
19	C	1.2807	72.32133	-1203.41001	-2.71241	-1206.12241	-1133.80108
20	C	1.2793	72.32867	-1202.15711	-2.71046	-1204.86757	-1132.53890
21	H	-0.0430	25.05800	10.16223	-0.22911	9.93312	34.99112
C Average		1.2807	72.32087	-1203.44133	-2.71330	-1206.15463	-1133.83376
H Average		-0.0446	25.05777	10.53248	-0.22955	10.30293	35.36070

```

=====
6MnCp2-STO-PBE-No-ZFS
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-66.186 0.000 -0.003
0.000 -66.186 0.001
-0.003 0.001 -68.566
-3.959 0.000 0.000
0.000 -3.959 0.000
0.000 0.000 -4.989

```

```

atensor 2 H
-2.315 -1.478 -1.181
-1.478 1.318 3.323
-1.181 3.323 0.897
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

```

```

atensor 3 C
-0.321 -0.236 -0.618
-0.236 0.260 1.739
-0.618 1.739 4.138
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

```


atensor 4 H
1.840 0.128 -3.526
0.128 -2.837 -0.096
-3.526 -0.096 0.897
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.343 0.020 -1.845
0.020 -0.404 -0.050
-1.845 -0.050 4.139
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.465 1.271 -0.998
1.271 1.469 -3.384
-0.998 -3.384 0.899
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.346 0.203 -0.522
0.203 0.283 -1.770
-0.522 -1.770 4.137
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.348 -2.184 2.910
-2.184 -1.341 -1.995
2.910 -1.995 0.900
0.001 -0.001 0.002
-0.001 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.103 -0.349 1.523
-0.349 -0.167 -1.044
1.523 -1.044 4.134
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.103 2.264 2.796
2.264 -1.098 2.151
2.796 2.151 0.899
0.001 0.001 0.002
0.001 0.000 0.002
0.000 0.000 0.000

atensor 11 C
0.064 0.362 1.463
0.362 -0.128 1.126
1.463 1.126 4.135
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.464 1.270 0.998
1.270 1.470 3.384

0.998 3.384 0.900
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.346 0.203 0.522
0.203 0.282 1.770
0.522 1.770 4.136
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.346 -2.184 -2.910
-2.184 -1.344 1.994
-2.910 1.994 0.898
0.001 -0.001 -0.002
-0.001 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.104 -0.349 -1.523
-0.349 -0.166 1.043
-1.523 1.043 4.139
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.101 2.264 -2.795
2.264 -1.099 -2.151
-2.795 -2.151 0.897
0.001 0.001 -0.002
0.001 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
0.065 0.362 -1.463
0.362 -0.126 -1.126
-1.463 -1.126 4.139
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.314 -1.479 1.182
-1.479 1.319 -3.324
1.182 -3.324 0.898
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.322 -0.236 0.618
-0.236 0.259 -1.740
0.618 -1.740 4.136
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.342 0.020 1.846
0.020 -0.406 0.050
1.846 0.050 4.134
0.009 0.000 0.003
0.000 0.003 0.000

-0.003 0.000 -0.001

atensor 21 H

1.842 0.128 3.527
0.128 -2.835 0.096
3.527 0.096 0.900
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn

-2937.329 -0.082 0.276
-0.082 -2937.497 -0.136
0.276 -0.136 -161.436
1937.059 0.000 0.002
0.000 1937.059 0.001
0.002 0.001 1933.666

orbtensor 2 H

-0.129 5.192 1.235
5.192 -12.889 -3.474
1.235 -3.474 -0.732
26.380 -4.232 -1.366
-4.232 36.782 3.843
-1.366 3.843 25.592

orbtensor 3 C

-177.411 22.665 8.345
22.665 -233.118 -23.467
8.345 -23.467 -61.192
227.430 -4.405 -3.902
-4.405 238.255 10.973
-3.902 10.973 224.557

orbtensor 4 H

-14.722 -0.450 3.686
-0.450 1.705 0.101
3.686 0.101 -0.732
38.276 0.367 -4.077
0.367 24.886 -0.111
-4.077 -0.111 25.592

orbtensor 5 C

-241.123 -1.963 24.900
-1.963 -169.410 0.680
24.900 0.680 -61.191
239.812 0.381 -11.641
0.381 225.876 -0.318
-11.641 -0.318 224.557

orbtensor 6 H

0.400 -4.464 1.043
-4.464 -13.417 3.536
1.043 3.536 -0.732
25.949 3.639 -1.154
3.639 37.212 -3.912
-1.154 -3.912 25.592

orbtensor 7 C

-175.096 -19.489 7.050
-19.489 -235.412 23.885
7.050 23.885 -61.191
226.981 3.787 -3.296
3.787 238.702 -11.169
-3.296 -11.169 224.559

orbtensor 8 H

-9.472	7.671	-3.041
7.671	-3.541	2.085
-3.041	2.085	-0.732
33.997	-6.254	3.363
-6.254	29.162	-2.306
3.363	-2.306	25.592

orbtensor 9 C

-218.185	33.486	-20.533
33.486	-192.300	14.079
-20.533	14.079	-61.191
235.353	-6.508	9.605
-6.508	230.321	-6.585
9.605	-6.585	224.561

orbtensor 10 H

-8.617	-7.950	-2.922
-7.950	-4.398	-2.248
-2.922	-2.248	-0.732
33.300	6.481	3.232
6.481	29.860	2.487
3.232	2.487	25.592

orbtensor 11 C

-214.457	-34.703	-19.733
-34.703	-196.043	-15.184
-19.733	-15.184	-61.191
234.627	6.745	9.229
6.745	231.049	7.102
9.229	7.102	224.559

orbtensor 12 H

0.402	-4.461	-1.043
-4.461	-13.417	-3.538
-1.043	-3.538	-0.733
25.947	3.637	1.153
3.637	37.213	3.913
1.153	3.913	25.593

orbtensor 13 C

-175.083	-19.473	-7.031
-19.473	-235.408	-23.903
-7.031	-23.903	-61.196
226.979	3.784	3.291
3.784	238.700	11.172
3.291	11.172	224.563

orbtensor 14 H

-9.477	7.671	3.043
7.671	-3.540	-2.085
3.043	-2.085	-0.733
34.001	-6.253	-3.365
-6.253	29.161	2.306
-3.365	2.306	25.593

orbtensor 15 C

-218.222	33.484	20.560
33.484	-192.303	-14.094
20.560	-14.094	-61.197
235.363	-6.506	-9.608
-6.506	230.324	6.583
-9.608	6.583	224.560

orbtensor 16 H

-8.616	-7.951	2.922
-7.951	-4.402	2.249
2.922	2.249	-0.732

```

33.299    6.482   -3.232
6.482    29.863  -2.487
-3.232   -2.487   25.592

```

```

orbtensor 17 C
-214.468  -34.713  19.749
-34.713  -196.071  15.176
19.749    15.176  -61.190
234.629    6.746  -9.231
6.746   231.055  -7.101
-9.231   -7.101  224.556

```

```

orbtensor 18 H
-0.129    5.193   -1.235
5.193   -12.888   3.472
-1.235    3.472   -0.731
26.380   -4.234    1.365
-4.234   36.781   -3.841
1.365   -3.841   25.591

```

```

orbtensor 19 C
-177.407   22.670   -8.330
22.670  -233.108   23.445
-8.330   23.445  -61.185
227.426   -4.406    3.899
-4.406   238.252  -10.972
3.899   -10.972  224.555

```

```

orbtensor 20 C
-241.090  -1.972  -24.876
-1.972 -169.392  -0.696
-24.876  -0.696  -61.188
239.804    0.382  11.640
0.382   225.869    0.320
11.640    0.320  224.559

```

```

orbtensor 21 H
-14.720  -0.452  -3.684
-0.452   1.706  -0.101
-3.684  -0.101  -0.731
38.275    0.368   4.076
0.368   24.885    0.112
4.076    0.112   25.592

```

```

gtensor (ppt)
-0.120  0.000  0.000
0.000  -0.120  0.000
0.000  0.000  -0.160
1.282  0.000  0.000
0.000  1.283  0.000
0.000  0.000  -0.135

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-71.2817	-76.15933	67816.43280	-0.52460	67815.90820	67739.74887
2	H	-0.0330	25.00133	7.79866	0.05324	7.85190	32.85323
3	C	1.3627	72.84033	-1280.42097	0.63226	-1279.78871	-1206.94838
4	H	-0.0330	25.00167	7.79866	0.05340	7.85206	32.85373
5	C	1.3630	72.84033	-1280.73419	0.63252	-1280.10167	-1207.26133
6	H	-0.0320	25.00133	7.56234	0.05329	7.61563	32.61696
7	C	1.3617	72.84767	-1279.48133	0.63226	-1278.84907	-1206.00140

8	H	-0.0307	25.00200	7.24724	0.05338	7.30062	32.30262
9	C	1.3603	72.85300	-1278.22847	0.63195	-1277.59652	-1204.74352
10	H	-0.0317	25.00167	7.48357	0.05337	7.53694	32.53860
11	C	1.3607	72.84800	-1278.54168	0.63210	-1277.90959	-1205.06159
12	H	-0.0310	25.00167	7.32602	0.05329	7.37931	32.38097
13	C	1.3610	72.85167	-1278.85490	0.63218	-1278.22272	-1205.37105
14	H	-0.0330	25.00167	7.79866	0.05340	7.85206	32.85373
15	C	1.3627	72.84167	-1280.42097	0.63256	-1279.78841	-1206.94675
16	H	-0.0333	25.00133	7.87744	0.05335	7.93079	32.93212
17	C	1.3630	72.83700	-1280.73419	0.63248	-1280.10171	-1207.26471
18	H	-0.0320	25.00133	7.56234	0.05324	7.61558	32.61691
19	C	1.3613	72.84433	-1279.16811	0.63211	-1278.53600	-1205.69167
20	C	1.3603	72.85400	-1278.22847	0.63199	-1277.59648	-1204.74248
21	H	-0.0307	25.00233	7.24724	0.05344	7.30068	32.30301
C Average		1.3617	72.84580	-1279.48133	0.63224	-1278.84909	-1206.00329
H Average		-0.0320	25.00163	7.57022	0.05334	7.62356	32.62519

=====
6MnCp2-STO-PBE-Neese
Temperature: 390
Spin: 2.5

atensor 1 Mn
-66.186 0.000 -0.003
0.000 -66.186 0.001
-0.003 0.001 -68.566
-3.959 0.000 0.000
0.000 -3.959 0.000
0.000 0.000 -4.989

atensor 2 H
-2.315 -1.478 -1.181
-1.478 1.318 3.323
-1.181 3.323 0.897
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C
-0.321 -0.236 -0.618
-0.236 0.260 1.739
-0.618 1.739 4.138
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H
1.840 0.128 -3.526
0.128 -2.837 -0.096
-3.526 -0.096 0.897
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.343 0.020 -1.845
0.020 -0.404 -0.050
-1.845 -0.050 4.139
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.465 1.271 -0.998
1.271 1.469 -3.384
-0.998 -3.384 0.899

-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.346 0.203 -0.522
0.203 0.283 -1.770
-0.522 -1.770 4.137
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.348 -2.184 2.910
-2.184 -1.341 -1.995
2.910 -1.995 0.900
0.001 -0.001 0.002
-0.001 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.103 -0.349 1.523
-0.349 -0.167 -1.044
1.523 -1.044 4.134
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.103 2.264 2.796
2.264 -1.098 2.151
2.796 2.151 0.899
0.001 0.001 0.002
0.001 0.000 0.002
0.000 0.000 0.000

atensor 11 C
0.064 0.362 1.463
0.362 -0.128 1.126
1.463 1.126 4.135
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.464 1.270 0.998
1.270 1.470 3.384
0.998 3.384 0.900
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.346 0.203 0.522
0.203 0.282 1.770
0.522 1.770 4.136
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.346 -2.184 -2.910
-2.184 -1.344 1.994
-2.910 1.994 0.898
0.001 -0.001 -0.002
-0.001 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.104 -0.349 -1.523
-0.349 -0.166 1.043
-1.523 1.043 4.139
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.101 2.264 -2.795
2.264 -1.099 -2.151
-2.795 -2.151 0.897
0.001 0.001 -0.002
0.001 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
0.065 0.362 -1.463
0.362 -0.126 -1.126
-1.463 -1.126 4.139
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.314 -1.479 1.182
-1.479 1.319 -3.324
1.182 -3.324 0.898
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.322 -0.236 0.618
-0.236 0.259 -1.740
0.618 -1.740 4.136
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.342 0.020 1.846
0.020 -0.406 0.050
1.846 0.050 4.134
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.842 0.128 3.527
0.128 -2.835 0.096
3.527 0.096 0.900
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2937.329 -0.082 0.276
-0.082 -2937.497 -0.136
0.276 -0.136 -161.436
1937.059 0.000 0.002
0.000 1937.059 0.001
0.002 0.001 1933.666

orbtensor 2 H
-0.129 5.192 1.235

5.192	-12.889	-3.474
1.235	-3.474	-0.732
26.380	-4.232	-1.366
-4.232	36.782	3.843
-1.366	3.843	25.592

orbtensor 3 C

-177.411	22.665	8.345
22.665	-233.118	-23.467
8.345	-23.467	-61.192
227.430	-4.405	-3.902
-4.405	238.255	10.973
-3.902	10.973	224.557

orbtensor 4 H

-14.722	-0.450	3.686
-0.450	1.705	0.101
3.686	0.101	-0.732
38.276	0.367	-4.077
0.367	24.886	-0.111
-4.077	-0.111	25.592

orbtensor 5 C

-241.123	-1.963	24.900
-1.963	-169.410	0.680
24.900	0.680	-61.191
239.812	0.381	-11.641
0.381	225.876	-0.318
-11.641	-0.318	224.557

orbtensor 6 H

0.400	-4.464	1.043
-4.464	-13.417	3.536
1.043	3.536	-0.732
25.949	3.639	-1.154
3.639	37.212	-3.912
-1.154	-3.912	25.592

orbtensor 7 C

-175.096	-19.489	7.050
-19.489	-235.412	23.885
7.050	23.885	-61.191
226.981	3.787	-3.296
3.787	238.702	-11.169
-3.296	-11.169	224.559

orbtensor 8 H

-9.472	7.671	-3.041
7.671	-3.541	2.085
-3.041	2.085	-0.732
33.997	-6.254	3.363
-6.254	29.162	-2.306
3.363	-2.306	25.592

orbtensor 9 C

-218.185	33.486	-20.533
33.486	-192.300	14.079
-20.533	14.079	-61.191
235.353	-6.508	9.605
-6.508	230.321	-6.585
9.605	-6.585	224.561

orbtensor 10 H

-8.617	-7.950	-2.922
-7.950	-4.398	-2.248
-2.922	-2.248	-0.732
33.300	6.481	3.232

6.481 29.860 2.487
3.232 2.487 25.592

orbtensor 11 C
-214.457 -34.703 -19.733
-34.703 -196.043 -15.184
-19.733 -15.184 -61.191
234.627 6.745 9.229
6.745 231.049 7.102
9.229 7.102 224.559

orbtensor 12 H
0.402 -4.461 -1.043
-4.461 -13.417 -3.538
-1.043 -3.538 -0.733
25.947 3.637 1.153
3.637 37.213 3.913
1.153 3.913 25.593

orbtensor 13 C
-175.083 -19.473 -7.031
-19.473 -235.408 -23.903
-7.031 -23.903 -61.196
226.979 3.784 3.291
3.784 238.700 11.172
3.291 11.172 224.563

orbtensor 14 H
-9.477 7.671 3.043
7.671 -3.540 -2.085
3.043 -2.085 -0.733
34.001 -6.253 -3.365
-6.253 29.161 2.306
-3.365 2.306 25.593

orbtensor 15 C
-218.222 33.484 20.560
33.484 -192.303 -14.094
20.560 -14.094 -61.197
235.363 -6.506 -9.608
-6.506 230.324 6.583
-9.608 6.583 224.560

orbtensor 16 H
-8.616 -7.951 2.922
-7.951 -4.402 2.249
2.922 2.249 -0.732
33.299 6.482 -3.232
6.482 29.863 -2.487
-3.232 -2.487 25.592

orbtensor 17 C
-214.468 -34.713 19.749
-34.713 -196.071 15.176
19.749 15.176 -61.190
234.629 6.746 -9.231
6.746 231.055 -7.101
-9.231 -7.101 224.556

orbtensor 18 H
-0.129 5.193 -1.235
5.193 -12.888 3.472
-1.235 3.472 -0.731
26.380 -4.234 1.365
-4.234 36.781 -3.841
1.365 -3.841 25.591

```

orbtensor 19 C
-177.407  22.670  -8.330
22.670 -233.108  23.445
-8.330  23.445 -61.185
227.426  -4.406  3.899
-4.406  238.252 -10.972
3.899  -10.972  224.555

```

```

orbtensor 20 C
-241.090  -1.972  -24.876
-1.972 -169.392  -0.696
-24.876  -0.696  -61.188
239.804  0.382  11.640
0.382  225.869  0.320
11.640  0.320  224.559

```

```

orbtensor 21 H
-14.720  -0.452  -3.684
-0.452  1.706  -0.101
-3.684  -0.101  -0.731
38.275  0.368  4.076
0.368  24.885  0.112
4.076  0.112  25.592

```

```

gtensor (ppt)
-0.120  0.000  0.000
0.000 -0.120  0.000
0.000  0.000 -0.160
1.282  0.000  0.000
0.000  1.283  0.000
0.000  0.000 -0.135

```

```

zfstensor (cm-1)
0.123940  -0.000096  0.000076
-0.000096  0.124257  -0.000007
0.000076  -0.000007  -0.248197

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-71.2817	-76.15933	67816.33905	2.64601	67818.98506	67742.82572
2	H	-0.0330	25.00133	7.79865	-0.26836	7.53029	32.53162
3	C	1.3627	72.84033	-1280.41920	-3.18925	-1283.60845	-1210.76812
4	H	-0.0330	25.00167	7.79865	-0.27000	7.52865	32.53032
5	C	1.3630	72.84033	-1280.73242	-3.19148	-1283.92389	-1211.08356
6	H	-0.0320	25.00133	7.56233	-0.26899	7.29334	32.29467
7	C	1.3617	72.84767	-1279.47956	-3.18931	-1282.66886	-1209.82120
8	H	-0.0307	25.00200	7.24723	-0.26846	6.97877	31.98077
9	C	1.3603	72.85300	-1278.22670	-3.18634	-1281.41304	-1208.56004
10	H	-0.0317	25.00167	7.48356	-0.26926	7.21429	32.21596
11	C	1.3607	72.84800	-1278.53992	-3.18772	-1281.72764	-1208.87964
12	H	-0.0310	25.00167	7.32601	-0.26880	7.05721	32.05888
13	C	1.3610	72.85167	-1278.85313	-3.18852	-1282.04165	-1209.18998
14	H	-0.0330	25.00167	7.79865	-0.26943	7.52922	32.53089
15	C	1.3627	72.84167	-1280.41920	-3.19123	-1283.61043	-1210.76876
16	H	-0.0333	25.00133	7.87743	-0.26990	7.60752	32.60886
17	C	1.3630	72.83700	-1280.73242	-3.19117	-1283.92358	-1211.08658
18	H	-0.0320	25.00133	7.56233	-0.26794	7.29439	32.29572
19	C	1.3613	72.84433	-1279.16635	-3.18761	-1282.35396	-1209.50962
20	C	1.3603	72.85400	-1278.22670	-3.18673	-1281.41343	-1208.55943
21	H	-0.0307	25.00233	7.24723	-0.26920	6.97804	31.98037

C Average	1.3617	72.84580	-1279.47956	-3.18894	-1282.66849	-1209.82269
H Average	-0.0320	25.00163	7.57021	-0.26904	7.30117	32.30281

=====
6MnCp2-STO-PBE-ORCA
Temperature: 390
Spin: 2.5

atensor 1 Mn
-66.186 0.000 -0.003
0.000 -66.186 0.001
-0.003 0.001 -68.566
-3.959 0.000 0.000
0.000 -3.959 0.000
0.000 0.000 -4.989

atensor 2 H
-2.315 -1.478 -1.181
-1.478 1.318 3.323
-1.181 3.323 0.897
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C
-0.321 -0.236 -0.618
-0.236 0.260 1.739
-0.618 1.739 4.138
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H
1.840 0.128 -3.526
0.128 -2.837 -0.096
-3.526 -0.096 0.897
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.343 0.020 -1.845
0.020 -0.404 -0.050
-1.845 -0.050 4.139
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.465 1.271 -0.998
1.271 1.469 -3.384
-0.998 -3.384 0.899
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.346 0.203 -0.522
0.203 0.283 -1.770
-0.522 -1.770 4.137
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.348 -2.184 2.910
-2.184 -1.341 -1.995

2.910 -1.995 0.900
0.001 -0.001 0.002
-0.001 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.103 -0.349 1.523
-0.349 -0.167 -1.044
1.523 -1.044 4.134
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.103 2.264 2.796
2.264 -1.098 2.151
2.796 2.151 0.899
0.001 0.001 0.002
0.001 0.000 0.002
0.000 0.000 0.000

atensor 11 C
0.064 0.362 1.463
0.362 -0.128 1.126
1.463 1.126 4.135
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.464 1.270 0.998
1.270 1.470 3.384
0.998 3.384 0.900
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.346 0.203 0.522
0.203 0.282 1.770
0.522 1.770 4.136
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.346 -2.184 -2.910
-2.184 -1.344 1.994
-2.910 1.994 0.898
0.001 -0.001 -0.002
-0.001 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.104 -0.349 -1.523
-0.349 -0.166 1.043
-1.523 1.043 4.139
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.101 2.264 -2.795
2.264 -1.099 -2.151
-2.795 -2.151 0.897
0.001 0.001 -0.002
0.001 0.000 -0.002

0.000 0.000 0.000

atensor 17 C
0.065 0.362 -1.463
0.362 -0.126 -1.126
-1.463 -1.126 4.139
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.314 -1.479 1.182
-1.479 1.319 -3.324
1.182 -3.324 0.898
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.322 -0.236 0.618
-0.236 0.259 -1.740
0.618 -1.740 4.136
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.342 0.020 1.846
0.020 -0.406 0.050
1.846 0.050 4.134
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.842 0.128 3.527
0.128 -2.835 0.096
3.527 0.096 0.900
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2937.329 -0.082 0.276
-0.082 -2937.497 -0.136
0.276 -0.136 -161.436
1937.059 0.000 0.002
0.000 1937.059 0.001
0.002 0.001 1933.666

orbtensor 2 H
-0.129 5.192 1.235
5.192 -12.889 -3.474
1.235 -3.474 -0.732
26.380 -4.232 -1.366
-4.232 36.782 3.843
-1.366 3.843 25.592

orbtensor 3 C
-177.411 22.665 8.345
22.665 -233.118 -23.467
8.345 -23.467 -61.192
227.430 -4.405 -3.902
-4.405 238.255 10.973
-3.902 10.973 224.557

orbtensor 4 H

-14.722	-0.450	3.686
-0.450	1.705	0.101
3.686	0.101	-0.732
38.276	0.367	-4.077
0.367	24.886	-0.111
-4.077	-0.111	25.592

orbtensor 5 C

-241.123	-1.963	24.900
-1.963	-169.410	0.680
24.900	0.680	-61.191
239.812	0.381	-11.641
0.381	225.876	-0.318
-11.641	-0.318	224.557

orbtensor 6 H

0.400	-4.464	1.043
-4.464	-13.417	3.536
1.043	3.536	-0.732
25.949	3.639	-1.154
3.639	37.212	-3.912
-1.154	-3.912	25.592

orbtensor 7 C

-175.096	-19.489	7.050
-19.489	-235.412	23.885
7.050	23.885	-61.191
226.981	3.787	-3.296
3.787	238.702	-11.169
-3.296	-11.169	224.559

orbtensor 8 H

-9.472	7.671	-3.041
7.671	-3.541	2.085
-3.041	2.085	-0.732
33.997	-6.254	3.363
-6.254	29.162	-2.306
3.363	-2.306	25.592

orbtensor 9 C

-218.185	33.486	-20.533
33.486	-192.300	14.079
-20.533	14.079	-61.191
235.353	-6.508	9.605
-6.508	230.321	-6.585
9.605	-6.585	224.561

orbtensor 10 H

-8.617	-7.950	-2.922
-7.950	-4.398	-2.248
-2.922	-2.248	-0.732
33.300	6.481	3.232
6.481	29.860	2.487
3.232	2.487	25.592

orbtensor 11 C

-214.457	-34.703	-19.733
-34.703	-196.043	-15.184
-19.733	-15.184	-61.191
234.627	6.745	9.229
6.745	231.049	7.102
9.229	7.102	224.559

orbtensor 12 H

0.402	-4.461	-1.043
-4.461	-13.417	-3.538
-1.043	-3.538	-0.733

25.947	3.637	1.153
3.637	37.213	3.913
1.153	3.913	25.593

orbtensor 13 C

-175.083	-19.473	-7.031
-19.473	-235.408	-23.903
-7.031	-23.903	-61.196
226.979	3.784	3.291
3.784	238.700	11.172
3.291	11.172	224.563

orbtensor 14 H

-9.477	7.671	3.043
7.671	-3.540	-2.085
3.043	-2.085	-0.733
34.001	-6.253	-3.365
-6.253	29.161	2.306
-3.365	2.306	25.593

orbtensor 15 C

-218.222	33.484	20.560
33.484	-192.303	-14.094
20.560	-14.094	-61.197
235.363	-6.506	-9.608
-6.506	230.324	6.583
-9.608	6.583	224.560

orbtensor 16 H

-8.616	-7.951	2.922
-7.951	-4.402	2.249
2.922	2.249	-0.732
33.299	6.482	-3.232
6.482	29.863	-2.487
-3.232	-2.487	25.592

orbtensor 17 C

-214.468	-34.713	19.749
-34.713	-196.071	15.176
19.749	15.176	-61.190
234.629	6.746	-9.231
6.746	231.055	-7.101
-9.231	-7.101	224.556

orbtensor 18 H

-0.129	5.193	-1.235
5.193	-12.888	3.472
-1.235	3.472	-0.731
26.380	-4.234	1.365
-4.234	36.781	-3.841
1.365	-3.841	25.591

orbtensor 19 C

-177.407	22.670	-8.330
22.670	-233.108	23.445
-8.330	23.445	-61.185
227.426	-4.406	3.899
-4.406	238.252	-10.972
3.899	-10.972	224.555

orbtensor 20 C

-241.090	-1.972	-24.876
-1.972	-169.392	-0.696
-24.876	-0.696	-61.188
239.804	0.382	11.640
0.382	225.869	0.320
11.640	0.320	224.559


```

orbtensor 21 H
-14.720  -0.452  -3.684
-0.452   1.706  -0.101
-3.684  -0.101  -0.731
38.275   0.368   4.076
0.368   24.885   0.112
4.076   0.112  25.592

```

```

gtensor (ppt)
-0.120   0.000   0.000
0.000  -0.120   0.000
0.000   0.000  -0.160
1.282   0.000   0.000
0.000   1.283   0.000
0.000   0.000  -0.135

```

```

zfstensor (cm-1)
-1.048330  -0.000278   0.001176
-0.000278  -1.047725  -0.000302
0.001176   -0.000302  -0.616195

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-71.2817	-76.15933	67816.42750	-4.19526	67812.23224	67736.07290
2	H	-0.0330	25.00133	7.79866	0.42358	8.22225	33.22358
3	C	1.3627	72.84033	-1280.42087	5.04844	-1275.37243	-1202.53210
4	H	-0.0330	25.00167	7.79866	0.41736	8.21603	33.21769
5	C	1.3630	72.84033	-1280.73409	5.04106	-1275.69302	-1202.85269
6	H	-0.0320	25.00133	7.56234	0.42686	7.98920	32.99053
7	C	1.3617	72.84767	-1279.48123	5.05624	-1274.42499	-1201.57732
8	H	-0.0307	25.00200	7.24724	0.43478	7.68203	32.68403
9	C	1.3603	72.85300	-1278.22837	5.06956	-1273.15881	-1200.30581
10	H	-0.0317	25.00167	7.48357	0.43003	7.91359	32.91526
11	C	1.3607	72.84800	-1278.54158	5.06401	-1273.47757	-1200.62957
12	H	-0.0310	25.00167	7.32602	0.42742	7.75344	32.75511
13	C	1.3610	72.85167	-1278.85480	5.05681	-1273.79799	-1200.94633
14	H	-0.0330	25.00167	7.79866	0.41998	8.21864	33.22031
15	C	1.3627	72.84167	-1280.42087	5.04329	-1275.37758	-1202.53591
16	H	-0.0333	25.00133	7.87744	0.42007	8.29751	33.29884
17	C	1.3630	72.83700	-1280.73409	5.04665	-1275.68744	-1202.85044
18	H	-0.0320	25.00133	7.56234	0.43248	7.99482	32.99615
19	C	1.3613	72.84433	-1279.16801	5.06572	-1274.10229	-1201.25796
20	C	1.3603	72.85400	-1278.22837	5.06865	-1273.15972	-1200.30572
21	H	-0.0307	25.00233	7.24724	0.43298	7.68022	32.68255
C Average		1.3617	72.84580	-1279.48123	5.05604	-1274.42518	-1201.57938
H Average		-0.0320	25.00163	7.57022	0.42655	7.99677	32.99841

```

=====
6MnCp2-STO-PBE-Pederson
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-66.186 0.000 -0.003
0.000 -66.186 0.001
-0.003 0.001 -68.566
-3.959 0.000 0.000
0.000 -3.959 0.000
0.000 0.000 -4.989

```

atensor 2 H
-2.315 -1.478 -1.181
-1.478 1.318 3.323
-1.181 3.323 0.897
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C
-0.321 -0.236 -0.618
-0.236 0.260 1.739
-0.618 1.739 4.138
0.004 -0.002 -0.001
-0.002 0.008 0.003
0.001 -0.003 -0.001

atensor 4 H
1.840 0.128 -3.526
0.128 -2.837 -0.096
-3.526 -0.096 0.897
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.343 0.020 -1.845
0.020 -0.404 -0.050
-1.845 -0.050 4.139
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.465 1.271 -0.998
1.271 1.469 -3.384
-0.998 -3.384 0.899
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.346 0.203 -0.522
0.203 0.283 -1.770
-0.522 -1.770 4.137
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.348 -2.184 2.910
-2.184 -1.341 -1.995
2.910 -1.995 0.900
0.001 -0.001 0.002
-0.001 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.103 -0.349 1.523
-0.349 -0.167 -1.044
1.523 -1.044 4.134
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.103 2.264 2.796

2.264 -1.098 2.151
2.796 2.151 0.899
0.001 0.001 0.002
0.001 0.000 0.002
0.000 0.000 0.000

atensor 11 C
0.064 0.362 1.463
0.362 -0.128 1.126
1.463 1.126 4.135
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H
-2.464 1.270 0.998
1.270 1.470 3.384
0.998 3.384 0.900
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.346 0.203 0.522
0.203 0.282 1.770
0.522 1.770 4.136
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.346 -2.184 -2.910
-2.184 -1.344 1.994
-2.910 1.994 0.898
0.001 -0.001 -0.002
-0.001 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.104 -0.349 -1.523
-0.349 -0.166 1.043
-1.523 1.043 4.139
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.101 2.264 -2.795
2.264 -1.099 -2.151
-2.795 -2.151 0.897
0.001 0.001 -0.002
0.001 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
0.065 0.362 -1.463
0.362 -0.126 -1.126
-1.463 -1.126 4.139
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.314 -1.479 1.182
-1.479 1.319 -3.324
1.182 -3.324 0.898
-0.001 -0.001 0.001

-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.322 -0.236 0.618
-0.236 0.259 -1.740
0.618 -1.740 4.136
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.342 0.020 1.846
0.020 -0.406 0.050
1.846 0.050 4.134
0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.842 0.128 3.527
0.128 -2.835 0.096
3.527 0.096 0.900
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2937.329 -0.082 0.276
-0.082 -2937.497 -0.136
0.276 -0.136 -161.436
1937.059 0.000 0.002
0.000 1937.059 0.001
0.002 0.001 1933.666

orbtensor 2 H
-0.129 5.192 1.235
5.192 -12.889 -3.474
1.235 -3.474 -0.732
26.380 -4.232 -1.366
-4.232 36.782 3.843
-1.366 3.843 25.592

orbtensor 3 C
-177.411 22.665 8.345
22.665 -233.118 -23.467
8.345 -23.467 -61.192
227.430 -4.405 -3.902
-4.405 238.255 10.973
-3.902 10.973 224.557

orbtensor 4 H
-14.722 -0.450 3.686
-0.450 1.705 0.101
3.686 0.101 -0.732
38.276 0.367 -4.077
0.367 24.886 -0.111
-4.077 -0.111 25.592

orbtensor 5 C
-241.123 -1.963 24.900
-1.963 -169.410 0.680
24.900 0.680 -61.191
239.812 0.381 -11.641
0.381 225.876 -0.318
-11.641 -0.318 224.557

orbtensor 6 H
0.400 -4.464 1.043
-4.464 -13.417 3.536
1.043 3.536 -0.732
25.949 3.639 -1.154
3.639 37.212 -3.912
-1.154 -3.912 25.592

orbtensor 7 C
-175.096 -19.489 7.050
-19.489 -235.412 23.885
7.050 23.885 -61.191
226.981 3.787 -3.296
3.787 238.702 -11.169
-3.296 -11.169 224.559

orbtensor 8 H
-9.472 7.671 -3.041
7.671 -3.541 2.085
-3.041 2.085 -0.732
33.997 -6.254 3.363
-6.254 29.162 -2.306
3.363 -2.306 25.592

orbtensor 9 C
-218.185 33.486 -20.533
33.486 -192.300 14.079
-20.533 14.079 -61.191
235.353 -6.508 9.605
-6.508 230.321 -6.585
9.605 -6.585 224.561

orbtensor 10 H
-8.617 -7.950 -2.922
-7.950 -4.398 -2.248
-2.922 -2.248 -0.732
33.300 6.481 3.232
6.481 29.860 2.487
3.232 2.487 25.592

orbtensor 11 C
-214.457 -34.703 -19.733
-34.703 -196.043 -15.184
-19.733 -15.184 -61.191
234.627 6.745 9.229
6.745 231.049 7.102
9.229 7.102 224.559

orbtensor 12 H
0.402 -4.461 -1.043
-4.461 -13.417 -3.538
-1.043 -3.538 -0.733
25.947 3.637 1.153
3.637 37.213 3.913
1.153 3.913 25.593

orbtensor 13 C
-175.083 -19.473 -7.031
-19.473 -235.408 -23.903
-7.031 -23.903 -61.196
226.979 3.784 3.291
3.784 238.700 11.172
3.291 11.172 224.563

orbtensor 14 H
-9.477 7.671 3.043
7.671 -3.540 -2.085

3.043	-2.085	-0.733
34.001	-6.253	-3.365
-6.253	29.161	2.306
-3.365	2.306	25.593
orbtensor 15 C		
-218.222	33.484	20.560
33.484	-192.303	-14.094
20.560	-14.094	-61.197
235.363	-6.506	-9.608
-6.506	230.324	6.583
-9.608	6.583	224.560
orbtensor 16 H		
-8.616	-7.951	2.922
-7.951	-4.402	2.249
2.922	2.249	-0.732
33.299	6.482	-3.232
6.482	29.863	-2.487
-3.232	-2.487	25.592
orbtensor 17 C		
-214.468	-34.713	19.749
-34.713	-196.071	15.176
19.749	15.176	-61.190
234.629	6.746	-9.231
6.746	231.055	-7.101
-9.231	-7.101	224.556
orbtensor 18 H		
-0.129	5.193	-1.235
5.193	-12.888	3.472
-1.235	3.472	-0.731
26.380	-4.234	1.365
-4.234	36.781	-3.841
1.365	-3.841	25.591
orbtensor 19 C		
-177.407	22.670	-8.330
22.670	-233.108	23.445
-8.330	23.445	-61.185
227.426	-4.406	3.899
-4.406	238.252	-10.972
3.899	-10.972	224.555
orbtensor 20 C		
-241.090	-1.972	-24.876
-1.972	-169.392	-0.696
-24.876	-0.696	-61.188
239.804	0.382	11.640
0.382	225.869	0.320
11.640	0.320	224.559
orbtensor 21 H		
-14.720	-0.452	-3.684
-0.452	1.706	-0.101
-3.684	-0.101	-0.731
38.275	0.368	4.076
0.368	24.885	0.112
4.076	0.112	25.592
gtensor (ppt)		
-0.120	0.000	0.000
0.000	-0.120	0.000
0.000	0.000	-0.160
1.282	0.000	0.000
0.000	1.283	0.000

0.000 0.000 -0.135

zfstensor (cm-1)

0.094634 -0.000075 0.000067
-0.000075 0.094889 -0.000007
0.000067 -0.000007 -0.189522

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-71.2817	-76.15933	67816.36944	1.89596	67818.26540	67742.10607
2	H	-0.0330	25.00133	7.79866	-0.19229	7.60637	32.60770
3	C	1.3627	72.84033	-1280.41978	-2.28527	-1282.70505	-1209.86471
4	H	-0.0330	25.00167	7.79866	-0.19358	7.60507	32.60674
5	C	1.3630	72.84033	-1280.73299	-2.28701	-1283.02000	-1210.17966
6	H	-0.0320	25.00133	7.56233	-0.19274	7.36959	32.37093
7	C	1.3617	72.84767	-1279.48013	-2.28527	-1281.76540	-1208.91773
8	H	-0.0307	25.00200	7.24724	-0.19227	7.05496	32.05696
9	C	1.3603	72.85300	-1278.22728	-2.28297	-1280.51024	-1207.65724
10	H	-0.0317	25.00167	7.48356	-0.19291	7.29064	32.29231
11	C	1.3607	72.84800	-1278.54049	-2.28403	-1280.82452	-1207.97652
12	H	-0.0310	25.00167	7.32601	-0.19258	7.13343	32.13510
13	C	1.3610	72.85167	-1278.85370	-2.28466	-1281.13836	-1208.28670
14	H	-0.0330	25.00167	7.79866	-0.19312	7.60553	32.60720
15	C	1.3627	72.84167	-1280.41978	-2.28678	-1282.70656	-1209.86489
16	H	-0.0333	25.00133	7.87743	-0.19349	7.68394	32.68528
17	C	1.3630	72.83700	-1280.73299	-2.28673	-1283.01972	-1210.18272
18	H	-0.0320	25.00133	7.56233	-0.19191	7.37043	32.37176
19	C	1.3613	72.84433	-1279.16692	-2.28393	-1281.45085	-1208.60652
20	C	1.3603	72.85400	-1278.22728	-2.28326	-1280.51054	-1207.65654
21	H	-0.0307	25.00233	7.24724	-0.19284	7.05439	32.05673
C Average		1.3617	72.84580	-1279.48013	-2.28499	-1281.76512	-1208.91932
H Average		-0.0320	25.00163	7.57021	-0.19277	7.37744	32.37907

6MnCp2-STO-PBE-Van-Wullen

Temperature: 390

Spin: 2.5

atensor 1 Mn

-66.186 0.000 -0.003
0.000 -66.186 0.001
-0.003 0.001 -68.566
-3.959 0.000 0.000
0.000 -3.959 0.000
0.000 0.000 -4.989

atensor 2 H

-2.315 -1.478 -1.181
-1.478 1.318 3.323
-1.181 3.323 0.897
-0.001 -0.001 -0.001
-0.001 0.002 0.003
0.000 0.000 0.000

atensor 3 C

-0.321 -0.236 -0.618
-0.236 0.260 1.739
-0.618 1.739 4.138
0.004 -0.002 -0.001
-0.002 0.008 0.003

0.001 -0.003 -0.001

atensor 4 H
1.840 0.128 -3.526
0.128 -2.837 -0.096
-3.526 -0.096 0.897
0.002 0.000 -0.003
0.000 -0.001 0.000
0.000 0.000 0.000

atensor 5 C
0.343 0.020 -1.845
0.020 -0.404 -0.050
-1.845 -0.050 4.139
0.009 0.000 -0.003
0.000 0.003 0.000
0.003 0.000 -0.001

atensor 6 H
-2.465 1.271 -0.998
1.271 1.469 -3.384
-0.998 -3.384 0.899
-0.001 0.001 -0.001
0.001 0.002 -0.003
0.000 0.000 0.000

atensor 7 C
-0.346 0.203 -0.522
0.203 0.283 -1.770
-0.522 -1.770 4.137
0.003 0.002 -0.001
0.002 0.009 -0.003
0.001 0.003 -0.001

atensor 8 H
0.348 -2.184 2.910
-2.184 -1.341 -1.995
2.910 -1.995 0.900
0.001 -0.001 0.002
-0.001 0.000 -0.002
0.000 0.000 0.000

atensor 9 C
0.103 -0.349 1.523
-0.349 -0.167 -1.044
1.523 -1.044 4.134
0.007 -0.003 0.003
-0.003 0.005 -0.002
-0.002 0.002 -0.001

atensor 10 H
0.103 2.264 2.796
2.264 -1.098 2.151
2.796 2.151 0.899
0.001 0.001 0.002
0.001 0.000 0.002
0.000 0.000 0.000

atensor 11 C
0.064 0.362 1.463
0.362 -0.128 1.126
1.463 1.126 4.135
0.007 0.003 0.003
0.003 0.005 0.002
-0.002 -0.002 -0.001

atensor 12 H

-2.464 1.270 0.998
1.270 1.470 3.384
0.998 3.384 0.900
-0.001 0.001 0.001
0.001 0.002 0.003
0.000 0.000 0.000

atensor 13 C
-0.346 0.203 0.522
0.203 0.282 1.770
0.522 1.770 4.136
0.003 0.002 0.001
0.002 0.009 0.003
-0.001 -0.003 -0.001

atensor 14 H
0.346 -2.184 -2.910
-2.184 -1.344 1.994
-2.910 1.994 0.898
0.001 -0.001 -0.002
-0.001 0.000 0.002
0.000 0.000 0.000

atensor 15 C
0.104 -0.349 -1.523
-0.349 -0.166 1.043
-1.523 1.043 4.139
0.007 -0.003 -0.003
-0.003 0.005 0.002
0.002 -0.002 -0.001

atensor 16 H
0.101 2.264 -2.795
2.264 -1.099 -2.151
-2.795 -2.151 0.897
0.001 0.001 -0.002
0.001 0.000 -0.002
0.000 0.000 0.000

atensor 17 C
0.065 0.362 -1.463
0.362 -0.126 -1.126
-1.463 -1.126 4.139
0.007 0.003 -0.003
0.003 0.005 -0.002
0.002 0.002 -0.001

atensor 18 H
-2.314 -1.479 1.182
-1.479 1.319 -3.324
1.182 -3.324 0.898
-0.001 -0.001 0.001
-0.001 0.002 -0.003
0.000 0.000 0.000

atensor 19 C
-0.322 -0.236 0.618
-0.236 0.259 -1.740
0.618 -1.740 4.136
0.004 -0.002 0.001
-0.002 0.008 -0.003
-0.001 0.003 -0.001

atensor 20 C
0.342 0.020 1.846
0.020 -0.406 0.050
1.846 0.050 4.134

0.009 0.000 0.003
0.000 0.003 0.000
-0.003 0.000 -0.001

atensor 21 H
1.842 0.128 3.527
0.128 -2.835 0.096
3.527 0.096 0.900
0.002 0.000 0.003
0.000 -0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-2937.329 -0.082 0.276
-0.082 -2937.497 -0.136
0.276 -0.136 -161.436
1937.059 0.000 0.002
0.000 1937.059 0.001
0.002 0.001 1933.666

orbtensor 2 H
-0.129 5.192 1.235
5.192 -12.889 -3.474
1.235 -3.474 -0.732
26.380 -4.232 -1.366
-4.232 36.782 3.843
-1.366 3.843 25.592

orbtensor 3 C
-177.411 22.665 8.345
22.665 -233.118 -23.467
8.345 -23.467 -61.192
227.430 -4.405 -3.902
-4.405 238.255 10.973
-3.902 10.973 224.557

orbtensor 4 H
-14.722 -0.450 3.686
-0.450 1.705 0.101
3.686 0.101 -0.732
38.276 0.367 -4.077
0.367 24.886 -0.111
-4.077 -0.111 25.592

orbtensor 5 C
-241.123 -1.963 24.900
-1.963 -169.410 0.680
24.900 0.680 -61.191
239.812 0.381 -11.641
0.381 225.876 -0.318
-11.641 -0.318 224.557

orbtensor 6 H
0.400 -4.464 1.043
-4.464 -13.417 3.536
1.043 3.536 -0.732
25.949 3.639 -1.154
3.639 37.212 -3.912
-1.154 -3.912 25.592

orbtensor 7 C
-175.096 -19.489 7.050
-19.489 -235.412 23.885
7.050 23.885 -61.191
226.981 3.787 -3.296
3.787 238.702 -11.169
-3.296 -11.169 224.559

orbtensor 8 H
-9.472 7.671 -3.041
7.671 -3.541 2.085
-3.041 2.085 -0.732
33.997 -6.254 3.363
-6.254 29.162 -2.306
3.363 -2.306 25.592

orbtensor 9 C
-218.185 33.486 -20.533
33.486 -192.300 14.079
-20.533 14.079 -61.191
235.353 -6.508 9.605
-6.508 230.321 -6.585
9.605 -6.585 224.561

orbtensor 10 H
-8.617 -7.950 -2.922
-7.950 -4.398 -2.248
-2.922 -2.248 -0.732
33.300 6.481 3.232
6.481 29.860 2.487
3.232 2.487 25.592

orbtensor 11 C
-214.457 -34.703 -19.733
-34.703 -196.043 -15.184
-19.733 -15.184 -61.191
234.627 6.745 9.229
6.745 231.049 7.102
9.229 7.102 224.559

orbtensor 12 H
0.402 -4.461 -1.043
-4.461 -13.417 -3.538
-1.043 -3.538 -0.733
25.947 3.637 1.153
3.637 37.213 3.913
1.153 3.913 25.593

orbtensor 13 C
-175.083 -19.473 -7.031
-19.473 -235.408 -23.903
-7.031 -23.903 -61.196
226.979 3.784 3.291
3.784 238.700 11.172
3.291 11.172 224.563

orbtensor 14 H
-9.477 7.671 3.043
7.671 -3.540 -2.085
3.043 -2.085 -0.733
34.001 -6.253 -3.365
-6.253 29.161 2.306
-3.365 2.306 25.593

orbtensor 15 C
-218.222 33.484 20.560
33.484 -192.303 -14.094
20.560 -14.094 -61.197
235.363 -6.506 -9.608
-6.506 230.324 6.583
-9.608 6.583 224.560

orbtensor 16 H
-8.616 -7.951 2.922

```

-7.951   -4.402   2.249
 2.922    2.249  -0.732
33.299    6.482  -3.232
 6.482   29.863  -2.487
-3.232   -2.487  25.592

```

```

orbtensor 17 C
-214.468  -34.713   19.749
-34.713  -196.071   15.176
 19.749   15.176  -61.190
234.629    6.746  -9.231
 6.746   231.055  -7.101
-9.231   -7.101  224.556

```

```

orbtensor 18 H
-0.129    5.193  -1.235
 5.193  -12.888   3.472
-1.235    3.472  -0.731
26.380   -4.234   1.365
-4.234   36.781  -3.841
 1.365   -3.841  25.591

```

```

orbtensor 19 C
-177.407   22.670  -8.330
 22.670  -233.108  23.445
-8.330   23.445  -61.185
227.426   -4.406   3.899
-4.406   238.252  -10.972
 3.899  -10.972  224.555

```

```

orbtensor 20 C
-241.090  -1.972  -24.876
-1.972  -169.392  -0.696
-24.876  -0.696  -61.188
239.804    0.382  11.640
 0.382   225.869   0.320
11.640    0.320  224.559

```

```

orbtensor 21 H
-14.720  -0.452  -3.684
-0.452   1.706  -0.101
-3.684  -0.101  -0.731
38.275    0.368   4.076
 0.368   24.885   0.112
 4.076    0.112  25.592

```

```

gtensor (ppt)
-0.120    0.000    0.000
 0.000  -0.120    0.000
 0.000    0.000  -0.160
 1.282    0.000    0.000
 0.000    1.283    0.000
 0.000    0.000  -0.135

```

```

zfstensor (cm-1)
0.118292  -0.000094   0.000084
-0.000094   0.118611  -0.000009
0.000084  -0.000009  -0.236903

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
---	----	------------	---------------	-----------	-----------	--------------	---------

1	Mn	-71.2817	-76.15933	67816.34530	2.50161	67818.84690	67742.68757
2	H	-0.0330	25.00133	7.79865	-0.25372	7.54493	32.54626
3	C	1.3627	72.84033	-1280.41932	-3.01527	-1283.43459	-1210.59426
4	H	-0.0330	25.00167	7.79865	-0.25538	7.54327	32.54494
5	C	1.3630	72.84033	-1280.73253	-3.01750	-1283.75004	-1210.90970
6	H	-0.0320	25.00133	7.56233	-0.25430	7.30803	32.30937
7	C	1.3617	72.84767	-1279.47968	-3.01526	-1282.49494	-1209.64727
8	H	-0.0307	25.00200	7.24723	-0.25374	6.99350	31.99550
9	C	1.3603	72.85300	-1278.22682	-3.01230	-1281.23912	-1208.38612
10	H	-0.0317	25.00167	7.48356	-0.25454	7.22902	32.23068
11	C	1.3607	72.84800	-1278.54003	-3.01367	-1281.55370	-1208.70570
12	H	-0.0310	25.00167	7.32601	-0.25410	7.07191	32.07358
13	C	1.3610	72.85167	-1278.85325	-3.01449	-1281.86773	-1209.01607
14	H	-0.0330	25.00167	7.79865	-0.25481	7.54385	32.54551
15	C	1.3627	72.84167	-1280.41932	-3.01723	-1283.43655	-1210.59489
16	H	-0.0333	25.00133	7.87743	-0.25525	7.62218	32.62351
17	C	1.3630	72.83700	-1280.73253	-3.01715	-1283.74968	-1210.91268
18	H	-0.0320	25.00133	7.56233	-0.25324	7.30909	32.31042
19	C	1.3613	72.84433	-1279.16646	-3.01355	-1282.18001	-1209.33568
20	C	1.3603	72.85400	-1278.22682	-3.01268	-1281.23950	-1208.38550
21	H	-0.0307	25.00233	7.24723	-0.25446	6.99277	31.99510
C Average		1.3617	72.84580	-1279.47968	-3.01491	-1282.49459	-1209.64879
H Average		-0.0320	25.00163	7.57021	-0.25435	7.31585	32.31749

=====
6MnCp2-STO-PBE0-No-ZFS

Temperature: 390

Spin: 2.5

atensor 1 Mn

-129.044 0.000 0.000
0.000 -129.044 0.000
0.000 0.000 -123.891
-4.231 0.000 0.000
0.000 -4.231 0.000
0.000 0.000 -4.494

atensor 2 H

-2.259 -1.437 -1.219
-1.437 1.272 3.430
-1.219 3.430 0.945
0.001 0.001 0.000
0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 3 C

-0.123 -0.260 -0.629
-0.260 0.516 1.770
-0.629 1.770 3.780
0.000 -0.001 0.000
-0.001 0.004 0.001
0.001 -0.002 0.000

atensor 4 H

1.779 0.124 -3.639
0.124 -2.767 -0.099
-3.639 -0.099 0.945
-0.001 0.000 0.001
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C

0.608 0.022 -1.878
0.022 -0.215 -0.051
-1.878 -0.051 3.781
0.004 0.000 -0.001

0.000 0.000 0.000
0.003 0.000 0.000

atensor 6 H
-2.405 1.235 -1.030
1.235 1.419 -3.492
-1.030 -3.492 0.946
0.001 0.000 0.000
0.000 -0.001 0.001
0.000 0.001 0.000

atensor 7 C
-0.150 0.224 -0.532
0.224 0.542 -1.802
-0.532 -1.802 3.779
0.000 0.001 0.000
0.001 0.004 -0.001
0.001 0.003 0.000

atensor 8 H
0.329 -2.123 3.004
-2.123 -1.312 -2.059
3.004 -2.059 0.947
0.000 0.001 -0.001
0.001 0.000 0.000
-0.001 0.000 0.000

atensor 9 C
0.344 -0.385 1.550
-0.385 0.047 -1.062
1.550 -1.062 3.777
0.003 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.092 2.200 2.886
2.200 -1.076 2.220
2.886 2.220 0.946
0.000 -0.001 0.000
-0.001 0.000 0.000
-0.001 0.000 0.000

atensor 11 C
0.302 0.399 1.489
0.399 0.090 1.146
1.489 1.146 3.777
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.002 0.000

atensor 12 H
-2.404 1.235 1.030
1.235 1.420 3.493
1.030 3.493 0.947
0.001 0.000 0.000
0.000 -0.001 -0.001
0.000 -0.001 0.000

atensor 13 C
-0.151 0.224 0.531
0.224 0.542 1.802
0.531 1.802 3.778
0.000 0.001 0.000
0.001 0.004 0.001
-0.001 -0.003 0.000

atensor 14 H
0.328 -2.122 -3.003
-2.122 -1.316 2.058
-3.003 2.058 0.946
0.000 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.000

atensor 15 C
0.345 -0.384 -1.550
-0.384 0.048 1.061
-1.550 1.061 3.781
0.003 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.089 2.200 -2.885
2.200 -1.077 -2.220
-2.885 -2.220 0.944
0.000 -0.001 0.000
-0.001 0.000 0.000
0.001 0.000 0.000

atensor 17 C
0.302 0.399 -1.489
0.399 0.091 -1.146
-1.489 -1.146 3.780
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.002 0.000

atensor 18 H
-2.258 -1.437 1.220
-1.437 1.273 -3.431
1.220 -3.431 0.945
0.001 0.001 0.000
0.001 -0.001 0.001
0.000 0.001 0.000

atensor 19 C
-0.124 -0.260 0.629
-0.260 0.516 -1.771
0.629 -1.771 3.778
0.000 -0.001 0.000
-0.001 0.004 -0.001
-0.001 0.002 0.000

atensor 20 C
0.608 0.022 1.878
0.022 -0.216 0.051
1.878 0.051 3.776
0.004 0.000 0.001
0.000 0.000 0.000
-0.003 0.000 0.000

atensor 21 H
1.782 0.125 3.640
0.125 -2.764 0.100
3.640 0.100 0.947
-0.001 0.000 -0.001
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1746.056 -0.043 0.209
-0.043 -1746.140 -0.082

```
0.209   -0.082  -95.184
1923.367  0.000   0.002
0.000  1923.368   0.000
0.002    0.000  1930.750
```

```
orbtensor 2 H
-1.839   5.589   0.655
5.589  -15.575  -1.842
0.655  -1.842  -0.357
27.970  -5.047  -0.919
-5.047  40.373   2.583
-0.919   2.583  25.113
```

```
orbtensor 3 C
-207.505  16.394   5.216
16.394 -247.801 -14.661
5.216 -14.661 -66.839
257.796   2.394  -1.087
2.394  251.910   3.051
-1.087   3.051  233.770
```

```
orbtensor 4 H
-17.548  -0.484   1.954
-0.484   0.135   0.054
1.954   0.054  -0.357
42.155   0.437  -2.741
0.437  26.188  -0.075
-2.741  -0.075  25.112
```

```
orbtensor 5 C
-253.588  -1.421  15.559
-1.421 -201.715   0.425
15.559   0.425 -66.838
251.065  -0.207  -3.238
-0.207  258.640  -0.088
-3.238  -0.088  233.769
```

```
orbtensor 6 H
-1.270  -4.805   0.553
-4.805 -16.144   1.875
0.553   1.875  -0.357
27.456   4.339  -0.776
4.339  40.888  -2.630
-0.776  -2.630  25.112
```

```
orbtensor 7 C
-205.825  -14.099   4.406
-14.099 -249.457  14.921
4.406  14.921 -66.837
258.038  -2.058  -0.918
-2.058  251.665  -3.106
-0.918  -3.106  233.770
```

```
orbtensor 8 H
-11.898   8.258  -1.611
8.258  -5.514   1.105
-1.611   1.105  -0.356
37.054  -7.458   2.261
-7.458  31.289  -1.550
2.261  -1.550  25.112
```

```
orbtensor 9 C
-236.995  24.223  -12.823
24.223 -218.271   8.794
-12.823   8.794 -66.836
253.482   3.539   2.670
3.539  256.219  -1.832
```



```

2.670    -1.832    233.770

orbtensor 10 H
-10.978   -8.558   -1.549
-8.558   -6.436   -1.191
-1.549   -1.191   -0.357
36.223    7.728    2.173
7.728   32.121    1.671
2.173    1.671    25.113

orbtensor 11 C
-234.302  -25.103  -12.324
-25.103  -220.982  -9.485
-12.324  -9.485  -66.837
253.879  -3.667    2.565
-3.667   255.826  1.975
2.565    1.975  233.771

orbtensor 12 H
-1.268   -4.803   -0.553
-4.803  -16.145  -1.876
-0.553  -1.876  -0.357
27.454   4.337   0.775
4.337   40.888   2.632
0.775    2.632   25.113

orbtensor 13 C
-205.813  -14.086  -4.387
-14.086  -249.453  -14.939
-4.387   -14.939  -66.839
258.038  -2.058    0.912
-2.058   251.663   3.109
0.912    3.109   233.771

orbtensor 14 H
-11.902    8.258    1.614
8.258   -5.511   -1.106
1.614   -1.106   -0.357
37.057   -7.457   -2.264
-7.457   31.286    1.551
-2.264    1.551   25.113

orbtensor 15 C
-237.022  24.222   12.851
24.222  -218.274  -8.813
12.851  -8.813  -66.841
253.484   3.538  -2.674
3.538   256.221  1.832
-2.674    1.832  233.770

orbtensor 16 H
-10.976   -8.559    1.549
-8.559   -6.438    1.192
1.549    1.192   -0.357
36.221    7.729   -2.173
7.729   32.123   -1.672
-2.173   -1.672   25.112

orbtensor 17 C
-234.311  -25.109   12.344
-25.109  -221.004   9.474
12.344   9.474  -66.838
253.881  -3.667  -2.570
-3.667   255.826  -1.971
-2.570   -1.971  233.769

orbtensor 18 H

```

```

-1.841    5.591    -0.654
5.591   -15.574    1.839
-0.654    1.839    -0.356
27.972   -5.048    0.917
-5.048   40.373   -2.581
0.917    -2.581   25.112

```

```

orbtensor 19 C
-207.504   16.398   -5.197
16.398  -247.796   14.637
-5.197   14.637  -66.835
257.794    2.395    1.081
2.395  251.912   -3.049
1.081   -3.049  233.769

```

```

orbtensor 20 C
-253.565   -1.427   -15.532
-1.427  -201.701   -0.442
-15.532   -0.442  -66.834
251.062   -0.209    3.235
-0.209  258.638    0.092
3.235    0.092  233.770

```

```

orbtensor 21 H
-17.547   -0.487   -1.952
-0.487    0.135   -0.054
-1.952   -0.054   -0.356
42.155    0.439    2.740
0.439   26.188    0.076
2.740    0.076   25.112

```

```

gtensor (ppt)
-0.142    0.000    0.000
0.000   -0.142    0.000
0.000    0.000   -0.164
-0.597    0.000    0.000
0.000   -0.597    0.000
0.000    0.000   -0.116

```

averaging
13C Average:3,5,7,9,11,13,15,17,19,20
1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-131.6450	730.03500	125166.35473	-0.23691	125166.11782	125896.15282
2	H	-0.0140	25.22833	3.30644	-0.01731	3.28913	28.51746
3	C	1.3923	73.77700	-1307.47233	-0.17138	-1307.64370	-1233.86670
4	H	-0.0143	25.22833	3.38516	-0.01732	3.36785	28.59618
5	C	1.3927	73.77767	-1307.78535	-0.17142	-1307.95677	-1234.17910
6	H	-0.0133	25.22833	3.14899	-0.01732	3.13167	28.36000
7	C	1.3917	73.78467	-1306.84629	-0.17135	-1307.01765	-1233.23298
8	H	-0.0120	25.22900	2.83409	-0.01731	2.81678	28.04578
9	C	1.3907	73.78967	-1305.90724	-0.17128	-1306.07852	-1232.28886
10	H	-0.0127	25.22867	2.99154	-0.01731	2.97423	28.20290
11	C	1.3907	73.78500	-1305.90724	-0.17128	-1306.07852	-1232.29352
12	H	-0.0123	25.22833	2.91281	-0.01732	2.89550	28.12383
13	C	1.3910	73.78900	-1306.22026	-0.17133	-1306.39159	-1232.60259
14	H	-0.0140	25.22867	3.30644	-0.01733	3.28911	28.51778
15	C	1.3927	73.77933	-1307.78535	-0.17142	-1307.95677	-1234.17744
16	H	-0.0147	25.22833	3.46389	-0.01731	3.44658	28.67492
17	C	1.3920	73.77433	-1307.15931	-0.17140	-1307.33071	-1233.55638
18	H	-0.0133	25.22867	3.14899	-0.01730	3.13169	28.36036
19	C	1.3913	73.78000	-1306.53328	-0.17130	-1306.70458	-1232.92458
20	C	1.3907	73.79000	-1305.90724	-0.17121	-1306.07845	-1232.28845

21	H	-0.0117	25.22900	2.75537	-0.01731	2.73806	27.96706
13C Average		1.3916	73.78267	-1306.75239	-0.17134	-1306.92373	-1233.14106
1H Average		-0.0132	25.22857	3.12537	-0.01731	3.10806	28.33663

=====
6MnCp2-STO-PBE0-ORCA
Temperature: 390
Spin: 2.5

atensor 1 Mn
-129.044 0.000 0.000
0.000 -129.044 0.000
0.000 0.000 -123.891
-4.231 0.000 0.000
0.000 -4.231 0.000
0.000 0.000 -4.494

atensor 2 H
-2.259 -1.437 -1.219
-1.437 1.272 3.430
-1.219 3.430 0.945
0.001 0.001 0.000
0.001 -0.001 -0.001
0.000 -0.001 0.000

atensor 3 C
-0.123 -0.260 -0.629
-0.260 0.516 1.770
-0.629 1.770 3.780
0.000 -0.001 0.000
-0.001 0.004 0.001
0.001 -0.002 0.000

atensor 4 H
1.779 0.124 -3.639
0.124 -2.767 -0.099
-3.639 -0.099 0.945
-0.001 0.000 0.001
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C
0.608 0.022 -1.878
0.022 -0.215 -0.051
-1.878 -0.051 3.781
0.004 0.000 -0.001
0.000 0.000 0.000
0.003 0.000 0.000

atensor 6 H
-2.405 1.235 -1.030
1.235 1.419 -3.492
-1.030 -3.492 0.946
0.001 0.000 0.000
0.000 -0.001 0.001
0.000 0.001 0.000

atensor 7 C
-0.150 0.224 -0.532
0.224 0.542 -1.802
-0.532 -1.802 3.779
0.000 0.001 0.000
0.001 0.004 -0.001
0.001 0.003 0.000

atensor 8 H

0.329 -2.123 3.004
-2.123 -1.312 -2.059
3.004 -2.059 0.947
0.000 0.001 -0.001
0.001 0.000 0.000
-0.001 0.000 0.000

atensor 9 C
0.344 -0.385 1.550
-0.385 0.047 -1.062
1.550 -1.062 3.777
0.003 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.092 2.200 2.886
2.200 -1.076 2.220
2.886 2.220 0.946
0.000 -0.001 0.000
-0.001 0.000 0.000
-0.001 0.000 0.000

atensor 11 C
0.302 0.399 1.489
0.399 0.090 1.146
1.489 1.146 3.777
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.002 0.000

atensor 12 H
-2.404 1.235 1.030
1.235 1.420 3.493
1.030 3.493 0.947
0.001 0.000 0.000
0.000 -0.001 -0.001
0.000 -0.001 0.000

atensor 13 C
-0.151 0.224 0.531
0.224 0.542 1.802
0.531 1.802 3.778
0.000 0.001 0.000
0.001 0.004 0.001
-0.001 -0.003 0.000

atensor 14 H
0.328 -2.122 -3.003
-2.122 -1.316 2.058
-3.003 2.058 0.946
0.000 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.000

atensor 15 C
0.345 -0.384 -1.550
-0.384 0.048 1.061
-1.550 1.061 3.781
0.003 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.089 2.200 -2.885
2.200 -1.077 -2.220
-2.885 -2.220 0.944

0.000 -0.001 0.000
-0.001 0.000 0.000
0.001 0.000 0.000

atensor 17 C
0.302 0.399 -1.489
0.399 0.091 -1.146
-1.489 -1.146 3.780
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.002 0.000

atensor 18 H
-2.258 -1.437 1.220
-1.437 1.273 -3.431
1.220 -3.431 0.945
0.001 0.001 0.000
0.001 -0.001 0.001
0.000 0.001 0.000

atensor 19 C
-0.124 -0.260 0.629
-0.260 0.516 -1.771
0.629 -1.771 3.778
0.000 -0.001 0.000
-0.001 0.004 -0.001
-0.001 0.002 0.000

atensor 20 C
0.608 0.022 1.878
0.022 -0.216 0.051
1.878 0.051 3.776
0.004 0.000 0.001
0.000 0.000 0.000
-0.003 0.000 0.000

atensor 21 H
1.782 0.125 3.640
0.125 -2.764 0.100
3.640 0.100 0.947
-0.001 0.000 -0.001
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1746.056 -0.043 0.209
-0.043 -1746.140 -0.082
0.209 -0.082 -95.184
1923.367 0.000 0.002
0.000 1923.368 0.000
0.002 0.000 1930.750

orbtensor 2 H
-1.839 5.589 0.655
5.589 -15.575 -1.842
0.655 -1.842 -0.357
27.970 -5.047 -0.919
-5.047 40.373 2.583
-0.919 2.583 25.113

orbtensor 3 C
-207.505 16.394 5.216
16.394 -247.801 -14.661
5.216 -14.661 -66.839
257.796 2.394 -1.087
2.394 251.910 3.051
-1.087 3.051 233.770

```

orbtensor 4 H
-17.548  -0.484   1.954
-0.484   0.135   0.054
1.954    0.054  -0.357
42.155   0.437  -2.741
0.437   26.188  -0.075
-2.741  -0.075   25.112

orbtensor 5 C
-253.588  -1.421   15.559
-1.421 -201.715   0.425
15.559    0.425  -66.838
251.065  -0.207  -3.238
-0.207  258.640  -0.088
-3.238  -0.088  233.769

orbtensor 6 H
-1.270  -4.805   0.553
-4.805 -16.144   1.875
0.553   1.875  -0.357
27.456   4.339  -0.776
4.339   40.888  -2.630
-0.776  -2.630   25.112

orbtensor 7 C
-205.825  -14.099   4.406
-14.099 -249.457  14.921
4.406   14.921 -66.837
258.038  -2.058  -0.918
-2.058  251.665  -3.106
-0.918  -3.106  233.770

orbtensor 8 H
-11.898   8.258  -1.611
8.258  -5.514   1.105
-1.611   1.105  -0.356
37.054  -7.458   2.261
-7.458  31.289  -1.550
2.261  -1.550   25.112

orbtensor 9 C
-236.995   24.223  -12.823
24.223 -218.271   8.794
-12.823   8.794 -66.836
253.482   3.539   2.670
3.539  256.219  -1.832
2.670  -1.832  233.770

orbtensor 10 H
-10.978  -8.558  -1.549
-8.558  -6.436  -1.191
-1.549  -1.191  -0.357
36.223   7.728   2.173
7.728  32.121   1.671
2.173   1.671   25.113

orbtensor 11 C
-234.302  -25.103  -12.324
-25.103 -220.982  -9.485
-12.324  -9.485 -66.837
253.879  -3.667   2.565
-3.667  255.826   1.975
2.565   1.975  233.771

orbtensor 12 H
-1.268  -4.803  -0.553

```

-4.803	-16.145	-1.876
-0.553	-1.876	-0.357
27.454	4.337	0.775
4.337	40.888	2.632
0.775	2.632	25.113

orbtensor 13 C

-205.813	-14.086	-4.387
-14.086	-249.453	-14.939
-4.387	-14.939	-66.839
258.038	-2.058	0.912
-2.058	251.663	3.109
0.912	3.109	233.771

orbtensor 14 H

-11.902	8.258	1.614
8.258	-5.511	-1.106
1.614	-1.106	-0.357
37.057	-7.457	-2.264
-7.457	31.286	1.551
-2.264	1.551	25.113

orbtensor 15 C

-237.022	24.222	12.851
24.222	-218.274	-8.813
12.851	-8.813	-66.841
253.484	3.538	-2.674
3.538	256.221	1.832
-2.674	1.832	233.770

orbtensor 16 H

-10.976	-8.559	1.549
-8.559	-6.438	1.192
1.549	1.192	-0.357
36.221	7.729	-2.173
7.729	32.123	-1.672
-2.173	-1.672	25.112

orbtensor 17 C

-234.311	-25.109	12.344
-25.109	-221.004	9.474
12.344	9.474	-66.838
253.881	-3.667	-2.570
-3.667	255.826	-1.971
-2.570	-1.971	233.769

orbtensor 18 H

-1.841	5.591	-0.654
5.591	-15.574	1.839
-0.654	1.839	-0.356
27.972	-5.048	0.917
-5.048	40.373	-2.581
0.917	-2.581	25.112

orbtensor 19 C

-207.504	16.398	-5.197
16.398	-247.796	14.637
-5.197	14.637	-66.835
257.794	2.395	1.081
2.395	251.912	-3.049
1.081	-3.049	233.769

orbtensor 20 C

-253.565	-1.427	-15.532
-1.427	-201.701	-0.442
-15.532	-0.442	-66.834
251.062	-0.209	3.235

-0.209 258.638 0.092
 3.235 0.092 233.770

orbtensor 21 H
 -17.547 -0.487 -1.952
 -0.487 0.135 -0.054
 -1.952 -0.054 -0.356
 42.155 0.439 2.740
 0.439 26.188 0.076
 2.740 0.076 25.112

gtensor (ppt)
 -0.142 0.000 0.000
 0.000 -0.142 0.000
 0.000 0.000 -0.164
 -0.597 0.000 0.000
 0.000 -0.597 0.000
 0.000 0.000 -0.116

zfstensor (cm-1)
 2.941115 0.357424 0.000859
 0.357424 -0.441964 -0.000235
 0.000859 -0.000235 -0.964597

averaging
 13C Average:3,5,7,9,11,13,15,17,19,20
 1H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-131.6450	730.03500	125158.17445	-27.12055	125131.05391	125861.08891
2	H	-0.0140	25.22833	3.30622	-8.41653	-5.11031	20.11802
3	C	1.3923	73.77700	-1307.38688	-24.28294	-1331.66982	-1257.89282
4	H	-0.0143	25.22833	3.38494	5.15930	8.54424	33.77258
5	C	1.3927	73.77767	-1307.69987	-14.46476	-1322.16464	-1248.38697
6	H	-0.0133	25.22833	3.14878	-7.11418	-3.96540	21.26293
7	C	1.3917	73.78467	-1306.76088	-23.33105	-1330.09194	-1256.30727
8	H	-0.0120	25.22900	2.83390	-0.81876	2.01514	27.24414
9	C	1.3907	73.78967	-1305.82190	-18.75815	-1324.58005	-1250.79038
10	H	-0.0127	25.22867	2.99134	1.28386	4.27520	29.50387
11	C	1.3907	73.78500	-1305.82190	-17.23523	-1323.05713	-1249.27213
12	H	-0.0123	25.22833	2.91262	-7.11405	-4.20142	21.02691
13	C	1.3910	73.78900	-1306.13489	-23.33422	-1329.46911	-1255.68011
14	H	-0.0140	25.22867	3.30622	-0.82688	2.47934	27.70801
15	C	1.3927	73.77933	-1307.69987	-18.79530	-1326.49518	-1252.71585
16	H	-0.0147	25.22833	3.46366	1.27358	4.73724	29.96558
17	C	1.3920	73.77433	-1307.07388	-17.26981	-1324.34369	-1250.56936
18	H	-0.0133	25.22867	3.14878	-8.40821	-5.25943	19.96924
19	C	1.3913	73.78000	-1306.44789	-24.26667	-1330.71456	-1256.93456
20	C	1.3907	73.79000	-1305.82190	-14.41043	-1320.23233	-1246.44233
21	H	-0.0117	25.22900	2.75519	5.17279	7.92798	33.15698
13C Average		1.3916	73.78267	-1306.66699	-19.61486	-1326.28184	-1252.49918
1H Average		-0.0132	25.22857	3.12517	-1.98091	1.14426	26.37283

=====
 6MnCp2-GTO-BP
 Temperature: 390
 Spin: 2.5

atensor 1 Mn
 -60.2321 0.0002 -0.0036
 0.0002 -60.2320 0.0002
 -0.0036 0.0002 -64.0893
 -3.4206 0.0000 0.0002

0.0000 -3.4206 0.0001
0.0002 0.0001 -4.5378

atensor 2 H
-2.2923 -1.4867 -1.1793
-1.4867 1.3616 3.3174
-1.1793 3.3174 0.8874
-0.0011 -0.0012 -0.0006
-0.0012 0.0019 0.0016
-0.0006 0.0016 0.0005

atensor 3 C
-0.4029 -0.2359 -0.6218
-0.2359 0.1770 1.7492
-0.6218 1.7492 4.1789
0.0035 -0.0020 -0.0001
-0.0020 0.0083 0.0004
-0.0001 0.0004 -0.0008

atensor 4 H
1.8865 0.1287 -3.5193
0.1287 -2.8173 -0.0961
-3.5193 -0.0961 0.8875
0.0023 0.0001 -0.0017
0.0001 -0.0016 -0.0000
-0.0017 -0.0000 0.0005

atensor 5 C
0.2602 0.0204 -1.8557
0.0204 -0.4862 -0.0506
-1.8557 -0.0506 4.1796
0.0090 0.0002 -0.0004
0.0002 0.0028 -0.0000
-0.0004 -0.0000 -0.0008

atensor 6 H
-2.4424 1.2781 -0.9963
1.2781 1.5142 -3.3774
-0.9963 -3.3774 0.8894
-0.0013 0.0011 -0.0005
0.0011 0.0020 -0.0016
-0.0005 -0.0016 0.0005

atensor 7 C
-0.4276 0.2029 -0.5254
0.2029 0.2003 -1.7806
-0.5254 -1.7806 4.1766
0.0033 0.0017 -0.0001
0.0017 0.0085 -0.0004
-0.0001 -0.0004 -0.0008

atensor 8 H
0.3861 -2.1968 2.9046
-2.1968 -1.3124 -1.9912
2.9046 -1.9912 0.8905
0.0011 -0.0018 0.0014
-0.0018 -0.0003 -0.0009
0.0014 -0.0009 0.0005

atensor 9 C
0.0206 -0.3487 1.5313
-0.3487 -0.2490 -1.0497
1.5313 -1.0497 4.1745
0.0070 -0.0029 0.0003
-0.0029 0.0048 -0.0002
0.0003 -0.0002 -0.0008

atensor 10 H
0.1399 2.2766 2.7910
2.2766 -1.0683 2.1472
2.7910 2.1472 0.8889
0.0009 0.0019 0.0013
0.0019 -0.0001 0.0010
0.0013 0.0010 0.0005

atensor 11 C
-0.0175 0.3614 1.4714
0.3614 -0.2092 1.1321
1.4714 1.1321 4.1761
0.0067 0.0030 0.0003
0.0030 0.0051 0.0003
0.0003 0.0003 -0.0008

atensor 12 H
-2.4432 1.2776 0.9957
1.2776 1.5137 3.3779
0.9957 3.3779 0.8898
-0.0013 0.0011 0.0005
0.0011 0.0020 0.0016
0.0005 0.0016 0.0005

atensor 13 C
-0.4268 0.2027 0.5249
0.2027 0.2009 1.7804
0.5249 1.7804 4.1773
0.0033 0.0017 0.0001
0.0017 0.0085 0.0004
0.0001 0.0004 -0.0008

atensor 14 H
0.3849 -2.1961 -2.9046
-2.1961 -1.3154 1.9899
-2.9046 1.9899 0.8889
0.0011 -0.0018 -0.0014
-0.0018 -0.0003 0.0009
-0.0014 0.0009 0.0005

atensor 15 C
0.0213 -0.3483 -1.5313
-0.3483 -0.2487 1.0486
-1.5313 1.0486 4.1786
0.0070 -0.0029 -0.0003
-0.0029 0.0048 0.0002
-0.0003 0.0002 -0.0008

atensor 16 H
0.1380 2.2768 -2.7898
2.2768 -1.0683 -2.1471
-2.7898 -2.1471 0.8872
0.0009 0.0019 -0.0013
0.0019 -0.0001 -0.0010
-0.0013 -0.0010 0.0005

atensor 17 C
-0.0178 0.3614 -1.4710
0.3614 -0.2090 -1.1324
-1.4710 -1.1324 4.1787
0.0067 0.0030 -0.0003
0.0030 0.0051 -0.0003
-0.0003 -0.0003 -0.0008

atensor 18 H
-2.2921 -1.4874 1.1794
-1.4874 1.3621 -3.3176

1.1794 -3.3176 0.8867
-0.0011 -0.0012 0.0006
-0.0012 0.0019 -0.0016
0.0006 -0.0016 0.0005

atensor 19 C
-0.4021 -0.2361 0.6219
-0.2361 0.1782 -1.7497
0.6219 -1.7497 4.1783
0.0035 -0.0020 0.0001
-0.0020 0.0083 -0.0004
0.0001 -0.0004 -0.0008

atensor 20 C
0.2583 0.0203 1.8561
0.0203 -0.4884 0.0504
1.8561 0.0504 4.1727
0.0090 0.0002 0.0004
0.0002 0.0028 0.0000
0.0004 0.0000 -0.0008

atensor 21 H
1.8896 0.1290 3.5204
0.1290 -2.8139 0.0963
3.5204 0.0963 0.8911
0.0024 0.0001 0.0017
0.0001 -0.0016 0.0000
0.0017 0.0000 0.0005

orbtensor 1 Mn
1930.4965 -0.0000 0.0027
-0.0000 1930.4966 -0.0003
0.0027 -0.0003 1938.5852
-3084.7795 -0.0329 0.2780
-0.0329 -3084.8317 -0.1728
0.2780 -0.1728 -170.7309

orbtensor 2 H
25.7414 -6.1475 -0.8469
-6.1475 40.8497 2.3822
-0.8469 2.3822 23.9537
1.0234 7.3024 0.7678
7.3024 -16.9218 -2.1605
0.7678 -2.1605 0.8114

orbtensor 3 C
257.8908 -0.0479 -0.4131
-0.0479 258.0045 1.1592
-0.4131 1.1592 240.2481
-216.7622 18.5815 5.0251
18.5815 -262.4166 -14.1214
5.0251 -14.1214 -83.1976

orbtensor 4 H
43.0208 0.5324 -2.5277
0.5324 23.5710 -0.0691
-2.5277 -0.0691 23.9536
-19.5011 -0.6324 2.2923
-0.6324 3.6020 0.0627
2.2923 0.0627 0.8116

orbtensor 5 C
258.0215 0.0039 -1.2309
0.0039 257.8723 -0.0335
-1.2309 -0.0335 240.2473
-268.9839 -1.6091 14.9886
-1.6091 -210.2007 0.4099

14.9886 0.4099 -83.2006

orbtensor 6 H

25.1155 5.2852 -0.7154
5.2852 41.4775 -2.4249
-0.7154 -2.4249 23.9540
1.7676 -6.2775 0.6484
-6.2775 -17.6668 2.1989
0.6484 2.1989 0.8120

orbtensor 7 C

257.8839 0.0411 -0.3494
0.0411 258.0089 -1.1789
-0.3494 -1.1789 240.2483
-214.8693 -15.9721 4.2436
-15.9721 -264.3057 14.3736
4.2436 14.3736 -83.1900

orbtensor 8 H

36.8077 -9.0846 2.0846
-9.0846 29.7842 -1.4293
2.0846 -1.4293 23.9539
-12.1193 10.7898 -1.8901
10.7898 -3.7775 1.2956
-1.8901 1.2956 0.8121

orbtensor 9 C

257.9731 -0.0697 1.0123
-0.0697 257.9194 -0.6946
1.0123 -0.6946 240.2495
-250.1758 27.4488 -12.3515
27.4488 -228.9630 8.4704
-12.3515 8.4704 -83.1978

orbtensor 10 H

35.7944 9.4139 2.0033
9.4139 30.7976 1.5412
2.0033 1.5412 23.9541
-10.9164 -11.1812 -1.8166
-11.1812 -4.9816 -1.3974
-1.8166 -1.3974 0.8119

orbtensor 11 C

257.9662 0.0721 0.9728
0.0721 257.9290 0.7501
0.9728 0.7501 240.2496
-247.1223 -28.4439 -11.8699
-28.4439 -232.0279 -9.1342
-11.8699 -9.1342 -83.1897

orbtensor 12 H

25.1137 5.2827 0.7148
5.2827 41.4781 2.4266
0.7148 2.4266 23.9544
1.7694 -6.2746 -0.6488
-6.2746 -17.6671 -2.2004
-0.6488 -2.2004 0.8116

orbtensor 13 C

257.8839 0.0400 0.3444
0.0400 258.0097 1.1812
0.3444 1.1812 240.2494
-214.8552 -15.9603 -4.2262
-15.9603 -264.2986 -14.3913
-4.2262 -14.3913 -83.1974

orbtensor 14 H

36.8107 -9.0828 -2.0877
-9.0828 29.7811 1.4304
-2.0877 1.4304 23.9540
-12.1241 10.7886 1.8933
10.7886 -3.7744 -1.2975
1.8933 -1.2975 0.8113

orbtensor 15 C
257.9746 -0.0693 -1.0175
-0.0693 257.9197 0.6972
-1.0175 0.6972 240.2473
-250.2125 27.4469 12.3810
27.4469 -228.9664 -8.4911
12.3810 -8.4911 -83.1988

orbtensor 16 H
35.7918 9.4145 -2.0038
9.4145 30.8005 -1.5414
-2.0038 -1.5414 23.9534
-10.9140 -11.1827 1.8168
-11.1827 -4.9855 1.3982
1.8168 1.3982 0.8116

orbtensor 17 C
257.9668 0.0722 -0.9780
0.0722 257.9281 -0.7479
-0.9780 -0.7479 240.2474
-247.1371 -28.4530 11.8908
-28.4530 -232.0525 9.1261
11.8908 9.1261 -83.1960

orbtensor 18 H
25.7427 -6.1494 0.8457
-6.1494 40.8495 -2.3796
0.8457 -2.3796 23.9534
1.0223 7.3042 -0.7672
7.3042 -16.9210 2.1573
-0.7672 2.1573 0.8121

orbtensor 19 C
257.8883 -0.0466 0.4088
-0.0466 258.0055 -1.1566
0.4088 -1.1566 240.2487
-216.7571 18.5824 -5.0062
18.5824 -262.4104 14.0970
-5.0062 14.0970 -83.1925

orbtensor 20 C
258.0215 0.0036 1.2255
0.0036 257.8721 0.0359
1.2255 0.0359 240.2505
-268.9572 -1.6157 -14.9596
-1.6157 -210.1896 -0.4259
-14.9596 -0.4259 -83.1935

orbtensor 21 H
43.0212 0.5351 2.5254
0.5351 23.5708 0.0695
2.5254 0.0695 23.9541
-19.4998 -0.6355 -2.2897
-0.6355 3.6021 -0.0628
-2.2897 -0.0628 0.8121

gtensor (ppt)
-0.0417 0.0000 0.0000
0.0000 -0.0417 0.0000
0.0000 0.0000 -0.0742

```

1.6664    0.0000    0.0004
0.0000    1.6664    0.0001
0.0004    0.0001   -0.1290

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-65.3108	-180.25460	62146.33740	-0.95976	62145.37764	61965.12304
2	H	-0.0140	25.15260	3.30908	0.06485	3.37393	28.52653
3	C	1.3213	64.58900	-1241.79234	0.81658	-1240.97575	-1176.38675
4	H	-0.0140	25.15263	3.31696	0.06496	3.38192	28.53455
5	C	1.3215	64.58530	-1241.98030	0.81694	-1241.16336	-1176.57806
6	H	-0.0125	25.15327	2.96242	0.06493	3.02735	28.18062
7	C	1.3201	64.59203	-1240.63325	0.81638	-1239.81687	-1175.22484
8	H	-0.0115	25.15370	2.71818	0.06480	2.78298	27.93668
9	C	1.3190	64.60180	-1239.63079	0.81580	-1238.81499	-1174.21319
10	H	-0.0127	25.15333	3.00969	0.06475	3.07444	28.22777
11	C	1.3201	64.60163	-1240.66458	0.81588	-1239.84869	-1175.24706
12	H	-0.0128	25.15337	3.03333	0.06487	3.09819	28.25156
13	C	1.3208	64.59727	-1241.29111	0.81614	-1240.47498	-1175.87771
14	H	-0.0134	25.15287	3.17514	0.06498	3.24012	28.39299
15	C	1.3207	64.58797	-1241.22846	0.81681	-1240.41165	-1175.82368
16	H	-0.0139	25.15260	3.29333	0.06492	3.35825	28.51085
17	C	1.3210	64.58557	-1241.44774	0.81683	-1240.63092	-1176.04535
18	H	-0.0140	25.15300	3.30908	0.06477	3.37386	28.52686
19	C	1.3218	64.59417	-1242.23091	0.81623	-1241.41468	-1176.82051
20	C	1.3179	64.60127	-1238.53436	0.81555	-1237.71881	-1173.11754
21	H	-0.0106	25.15350	2.51333	0.06475	2.57808	27.73158
C Average		1.3204	64.59360	-1240.94338	0.81631	-1240.12707	-1175.53347
H Average		-0.0130	25.15309	3.06405	0.06486	3.12891	28.28200

```

=====
6MnCp2-GTO-PBE
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-73.9790 0.0002 -0.0035
0.0002 -73.9786 0.0001
-0.0035 0.0001 -76.9962
-3.4268 0.0000 0.0002
0.0000 -3.4268 0.0001
0.0002 0.0001 -4.4325

```

```

atensor 2 H
-2.2852 -1.4821 -1.1831
-1.4821 1.3575 3.3280
-1.1831 3.3280 0.8929
-0.0009 -0.0011 -0.0005
-0.0011 0.0017 0.0014
-0.0005 0.0014 0.0005

```

```

atensor 3 C
-0.3278 -0.2376 -0.6210
-0.2376 0.2563 1.7470
-0.6210 1.7470 4.1869
0.0032 -0.0019 -0.0001
-0.0019 0.0080 0.0002
-0.0001 0.0002 -0.0007

```

```

atensor 4 H

```

1.8809 0.1283 -3.5306
0.1283 -2.8084 -0.0964
-3.5306 -0.0964 0.8932
0.0021 0.0001 -0.0014
0.0001 -0.0013 -0.0000
-0.0014 -0.0000 0.0005

atensor 5 C
0.3397 0.0205 -1.8534
0.0205 -0.4122 -0.0505
-1.8534 -0.0505 4.1871
0.0087 0.0002 -0.0003
0.0002 0.0025 -0.0000
-0.0003 -0.0000 -0.0007

atensor 6 H
-2.4362 1.2743 -0.9995
1.2743 1.5086 -3.3882
-0.9995 -3.3882 0.8936
-0.0010 0.0009 -0.0004
0.0009 0.0018 -0.0014
-0.0004 -0.0014 0.0005

atensor 7 C
-0.3514 0.2044 -0.5247
0.2044 0.2810 -1.7783
-0.5247 -1.7783 4.1865
0.0030 0.0017 -0.0001
0.0017 0.0082 -0.0002
-0.0001 -0.0002 -0.0007

atensor 8 H
0.3854 -2.1900 2.9139
-2.1900 -1.3079 -1.9976
2.9139 -1.9976 0.8964
0.0010 -0.0016 0.0012
-0.0016 -0.0002 -0.0008
0.0012 -0.0008 0.0005

atensor 9 C
0.0979 -0.3512 1.5294
-0.3512 -0.1737 -1.0484
1.5294 -1.0484 4.1817
0.0067 -0.0029 0.0002
-0.0029 0.0045 -0.0001
0.0002 -0.0001 -0.0007

atensor 10 H
0.1393 2.2697 2.7999
2.2697 -1.0653 2.1540
2.7999 2.1540 0.8941
0.0008 0.0017 0.0011
0.0017 -0.0000 0.0009
0.0011 0.0009 0.0005

atensor 11 C
0.0607 0.3640 1.4696
0.3640 -0.1324 1.1307
1.4696 1.1307 4.1846
0.0064 0.0030 0.0002
0.0030 0.0048 0.0002
0.0002 0.0002 -0.0007

atensor 12 H
-2.4341 1.2735 0.9989
1.2735 1.5103 3.3887
0.9989 3.3887 0.8967

-0.0010 0.0009 0.0004
0.0009 0.0018 0.0014
0.0004 0.0014 0.0005

atensor 13 C
-0.3542 0.2042 0.5243
0.2042 0.2781 1.7782
0.5243 1.7782 4.1823
0.0030 0.0017 0.0001
0.0017 0.0082 0.0002
0.0001 0.0002 -0.0007

atensor 14 H
0.3824 -2.1896 -2.9139
-2.1896 -1.3129 1.9962
-2.9139 1.9962 0.8927
0.0010 -0.0016 -0.0012
-0.0016 -0.0002 0.0008
-0.0012 0.0008 0.0005

atensor 15 C
0.1013 -0.3509 -1.5293
-0.3509 -0.1707 1.0474
-1.5293 1.0474 4.1892
0.0067 -0.0029 -0.0002
-0.0029 0.0045 0.0001
-0.0002 0.0001 -0.0007

atensor 16 H
0.1377 2.2699 -2.7988
2.2699 -1.0650 -2.1540
-2.7988 -2.1540 0.8927
0.0008 0.0016 -0.0011
0.0016 -0.0000 -0.0009
-0.0011 -0.0009 0.0005

atensor 17 C
0.0601 0.3641 -1.4691
0.3641 -0.1326 -1.1311
-1.4691 -1.1311 4.1868
0.0064 0.0030 -0.0002
0.0030 0.0048 -0.0002
-0.0002 -0.0002 -0.0007

atensor 18 H
-2.2837 -1.4827 1.1832
-1.4827 1.3590 -3.3282
1.1832 -3.3282 0.8934
-0.0009 -0.0011 0.0005
-0.0011 0.0017 -0.0014
0.0005 -0.0014 0.0005

atensor 19 C
-0.3286 -0.2378 0.6211
-0.2378 0.2559 -1.7475
0.6211 -1.7475 4.1842
0.0032 -0.0019 0.0001
-0.0019 0.0080 -0.0002
0.0001 -0.0002 -0.0007

atensor 20 C
0.3408 0.0204 1.8538
0.0204 -0.4114 0.0503
1.8538 0.0503 4.1845
0.0087 0.0002 0.0003
0.0002 0.0026 0.0000
0.0003 0.0000 -0.0007

atensor 21 H

1.8821 0.1286 3.5317
0.1286 -2.8078 0.0966
3.5317 0.0966 0.8941
0.0021 0.0001 0.0014
0.0001 -0.0013 0.0000
0.0014 0.0000 0.0005

orbtensor 1 Mn

1931.8525 -0.0000 0.0025
-0.0000 1931.8526 -0.0004
0.0025 -0.0004 1939.3338
-2973.3484 -0.0296 0.2699
-0.0296 -2973.3943 -0.1590
0.2699 -0.1590 -167.5288

orbtensor 2 H

25.5255 -5.9818 -0.8663
-5.9818 40.2264 2.4367
-0.8663 2.4367 24.0256
1.1345 7.1137 0.7729
7.1137 -16.3471 -2.1751
0.7729 -2.1751 0.6463

orbtensor 3 C

254.7875 -0.2657 -0.7427
-0.2657 255.4360 2.0869
-0.7427 2.0869 239.1116
-213.7835 18.7717 5.3381
18.7717 -259.9055 -15.0018
5.3381 -15.0018 -81.8509

orbtensor 4 H

42.3390 0.5181 -2.5855
0.5181 23.4137 -0.0708
-2.5855 -0.0708 24.0256
-18.8597 -0.6161 2.3077
-0.6161 3.6465 0.0632
2.3077 0.0632 0.6462

orbtensor 5 C

255.5295 0.0228 -2.2152
0.0228 254.6917 -0.0607
-2.2152 -0.0607 239.1104
-266.5405 -1.6258 15.9231
-1.6258 -207.1546 0.4356
15.9231 0.4356 -81.8535

orbtensor 6 H

24.9166 5.1426 -0.7318
5.1426 40.8373 -2.4804
-0.7318 -2.4804 24.0260
1.8593 -6.1153 0.6527
-6.1153 -17.0730 2.2138
0.6527 2.2138 0.6468

orbtensor 7 C

254.7585 0.2283 -0.6278
0.2283 255.4628 -2.1236
-0.6278 -2.1236 239.1117
-211.8711 -16.1359 4.5080
-16.1359 -261.8149 15.2698
4.5080 15.2698 -81.8427

orbtensor 8 H

36.2934 -8.8396 2.1324

-8.8396 29.4594 -1.4620
2.1324 -1.4620 24.0259
-11.6687 10.5110 -1.9029
10.5110 -3.5425 1.3045
-1.9029 1.3045 0.6468

orbtensor 9 C
255.2615 -0.3913 1.8246
-0.3913 254.9594 -1.2516
1.8246 -1.2516 239.1127
-247.5407 27.7309 -13.1226
27.7309 -226.1104 8.9989
-13.1226 8.9989 -81.8506

orbtensor 10 H
35.3075 9.1600 2.0492
9.1600 30.4454 1.5764
2.0492 1.5764 24.0261
-10.4968 -10.8923 -1.8289
-10.8923 -4.7155 -1.4068
-1.8289 -1.4068 0.6466

orbtensor 11 C
255.2190 0.4055 1.7534
0.4055 255.0047 1.3503
1.7534 1.3503 239.1128
-244.4557 -28.7357 -12.6107
-28.7357 -229.2062 -9.7039
-12.6107 -9.7039 -81.8427

orbtensor 12 H
24.9147 5.1402 0.7311
5.1402 40.8378 2.4820
0.7311 2.4820 24.0264
1.8611 -6.1124 -0.6533
-6.1124 -17.0730 -2.2152
-0.6533 -2.2152 0.6465

orbtensor 13 C
254.7580 0.2269 0.6230
0.2269 255.4632 2.1253
0.6230 2.1253 239.1132
-211.8562 -16.1241 -4.4903
-16.1241 -261.8065 -15.2872
-4.4903 -15.2872 -81.8508

orbtensor 14 H
36.2963 -8.8378 -2.1354
-8.8378 29.4563 1.4630
-2.1354 1.4630 24.0259
-11.6731 10.5097 1.9057
10.5097 -3.5393 -1.3061
1.9057 -1.3061 0.6457

orbtensor 15 C
255.2627 -0.3907 -1.8296
-0.3907 254.9584 1.2535
-1.8296 1.2535 239.1106
-247.5756 27.7281 13.1523
27.7281 -226.1111 -9.0190
13.1523 -9.0190 -81.8514

orbtensor 16 H
35.3050 9.1606 -2.0497
9.1606 30.4483 -1.5768
-2.0497 -1.5768 24.0254
-10.4945 -10.8938 1.8288

-10.8938 -4.7192 1.4077
 1.8288 1.4077 0.6458

orbtensor 17 C
 255.2193 0.4056 -1.7583
 0.4056 255.0039 -1.3488
 -1.7583 -1.3488 239.1104
 -244.4693 -28.7447 12.6319
 -28.7447 -229.2304 9.6965
 12.6319 9.6965 -81.8479

orbtensor 18 H
 25.5269 -5.9835 0.8651
 -5.9835 40.2264 -2.4342
 0.8651 -2.4342 24.0253
 1.1332 7.1155 -0.7724
 7.1155 -16.3466 2.1719
 -0.7724 2.1719 0.6468

orbtensor 19 C
 254.7856 -0.2643 0.7389
 -0.2643 255.4382 -2.0848
 0.7389 -2.0848 239.1118
 -213.7793 18.7731 -5.3193
 18.7731 -259.9012 14.9780
 -5.3193 14.9780 -81.8447

orbtensor 20 C
 255.5303 0.0224 2.2100
 0.0224 254.6922 0.0626
 2.2100 0.0626 239.1137
 -266.5157 -1.6321 -15.8941
 -1.6321 -207.1438 -0.4512
 -15.8941 -0.4512 -81.8465

orbtensor 21 H
 42.3394 0.5206 2.5833
 0.5206 23.4135 0.0711
 2.5833 0.0711 24.0260
 -18.8585 -0.6191 -2.3053
 -0.6191 3.6464 -0.0632
 -2.3053 -0.0632 0.6468

gtensor (ppt)
 -0.0411 -0.0000 0.0000
 -0.0000 -0.0411 0.0000
 0.0000 0.0000 -0.0740
 1.4613 0.0000 0.0004
 0.0000 1.4614 0.0001
 0.0004 0.0001 -0.1300

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-78.7466	-103.74420	74926.06482	-0.68973	74925.37510	74821.63090
2	H	-0.0112	25.07040	2.63921	0.05779	2.69699	27.76739
3	C	1.3753	64.59840	-1292.42224	0.71396	-1291.70828	-1227.10988
4	H	-0.0110	25.07043	2.59982	0.05791	2.65773	27.72816
5	C	1.3750	64.59433	-1292.17164	0.71430	-1291.45734	-1226.86301
6	H	-0.0109	25.07100	2.57618	0.05786	2.63404	27.70504
7	C	1.3755	64.60143	-1292.64151	0.71389	-1291.92762	-1227.32618
8	H	-0.0083	25.07143	1.95380	0.05775	2.01155	27.08298

9	C	1.3721	64.61063	-1289.44640	0.71326	-1288.73313	-1224.12250
10	H	-0.0102	25.07110	2.41074	0.05769	2.46843	27.53953
11	C	1.3745	64.61063	-1291.63912	0.71335	-1290.92577	-1226.31514
12	H	-0.0086	25.07117	2.03258	0.05780	2.09038	27.16155
13	C	1.3722	64.60697	-1289.54037	0.71342	-1288.82695	-1224.21998
14	H	-0.0122	25.07060	2.87555	0.05791	2.93347	28.00407
15	C	1.3768	64.59787	-1293.80052	0.71431	-1293.08621	-1228.48834
16	H	-0.0111	25.07027	2.62345	0.05787	2.68132	27.75159
17	C	1.3749	64.59533	-1292.07767	0.71423	-1291.36344	-1226.76811
18	H	-0.0100	25.07067	2.36347	0.05772	2.42119	27.49186
19	C	1.3740	64.60347	-1291.20058	0.71355	-1290.48702	-1225.88356
20	C	1.3748	64.61007	-1291.98369	0.71322	-1291.27047	-1226.66041
21	H	-0.0101	25.07120	2.38710	0.05769	2.44479	27.51599
C Average		1.3745	64.60291	-1291.69237	0.71375	-1290.97862	-1226.37571
H Average		-0.0104	25.07083	2.44619	0.05780	2.50399	27.57482

=====
6MnCP2-GTO-B3LYP

Temperature: 390

Spin: 2.5

atensor 1 Mn

-94.2471 0.0001 -0.0013
0.0001 -94.2469 -0.0003
-0.0013 -0.0003 -92.3132
-3.6248 0.0000 0.0002
0.0000 -3.6248 0.0000
0.0002 0.0000 -4.0575

atensor 2 H

-2.3118 -1.4816 -1.2075
-1.4816 1.3296 3.3966
-1.2075 3.3966 0.8447
-0.0001 -0.0003 -0.0001
-0.0003 0.0005 0.0004
-0.0001 0.0004 0.0004

atensor 3 C

-0.0630 -0.2581 -0.6293
-0.2581 0.5715 1.7702
-0.6293 1.7702 4.3023
0.0008 -0.0014 0.0002
-0.0014 0.0044 -0.0005
0.0002 -0.0005 -0.0006

atensor 4 H

1.8525 0.1282 -3.6034
0.1282 -2.8352 -0.0984
-3.6034 -0.0984 0.8447
0.0006 0.0000 -0.0004
0.0000 -0.0002 -0.0000
-0.0004 -0.0000 0.0004

atensor 5 C

0.6626 0.0223 -1.8780
0.0223 -0.1541 -0.0512
-1.8780 -0.0512 4.3027
0.0049 0.0001 0.0005
0.0001 0.0003 0.0000
0.0005 0.0000 -0.0006

atensor 6 H

-2.4618 1.2738 -1.0201
1.2738 1.4813 -3.4580
-1.0201 -3.4580 0.8463
-0.0002 0.0002 -0.0001

0.0002 0.0005 -0.0004
-0.0001 -0.0004 0.0004

atensor 7 C
-0.0899 0.2220 -0.5317
0.2220 0.5971 -1.8020
-0.5317 -1.8020 4.3000
0.0007 0.0012 0.0001
0.0012 0.0045 0.0005
0.0001 0.0005 -0.0006

atensor 8 H
0.3569 -2.1894 2.9740
-2.1894 -1.3358 -2.0388
2.9740 -2.0388 0.8473
0.0003 -0.0004 0.0003
-0.0004 0.0000 -0.0002
0.0003 -0.0002 0.0004

atensor 9 C
0.4007 -0.3815 1.5497
-0.3815 0.1057 -1.0624
1.5497 -1.0624 4.2983
0.0034 -0.0021 -0.0004
-0.0021 0.0018 0.0003
-0.0004 0.0003 -0.0006

atensor 10 H
0.1120 2.2688 2.8577
2.2688 -1.0921 2.1985
2.8577 2.1985 0.8462
0.0003 0.0004 0.0003
0.0004 0.0001 0.0003
0.0003 0.0003 0.0004

atensor 11 C
0.3585 0.3954 1.4891
0.3954 0.1488 1.1457
1.4891 1.1457 4.2994
0.0032 0.0022 -0.0004
0.0022 0.0020 -0.0003
-0.0004 -0.0003 -0.0006

atensor 12 H
-2.4617 1.2731 1.0195
1.2731 1.4815 3.4586
1.0195 3.4586 0.8477
-0.0002 0.0002 0.0001
0.0002 0.0005 0.0004
0.0001 0.0004 0.0004

atensor 13 C
-0.0902 0.2218 0.5312
0.2218 0.5966 1.8018
0.5312 1.8018 4.2997
0.0007 0.0012 -0.0001
0.0012 0.0045 -0.0005
-0.0001 -0.0005 -0.0006

atensor 14 H
0.3558 -2.1886 -2.9739
-2.1886 -1.3388 2.0374
-2.9739 2.0374 0.8457
0.0003 -0.0004 -0.0003
-0.0004 0.0000 0.0002
-0.0003 0.0002 0.0004

atensor 15 C
0.4016 -0.3812 -1.5497
-0.3812 0.1062 1.0613
-1.5497 1.0613 4.3025
0.0034 -0.0021 0.0004
-0.0021 0.0018 -0.0003
0.0004 -0.0003 -0.0006

atensor 16 H
0.1095 2.2691 -2.8565
2.2691 -1.0927 -2.1983
-2.8565 -2.1983 0.8439
0.0003 0.0004 -0.0003
0.0004 0.0001 -0.0003
-0.0003 -0.0003 0.0004

atensor 17 C
0.3590 0.3954 -1.4887
0.3954 0.1497 -1.1460
-1.4887 -1.1460 4.3025
0.0032 0.0022 0.0004
0.0022 0.0020 0.0003
0.0004 0.0003 -0.0006

atensor 18 H
-2.3108 -1.4822 1.2076
-1.4822 1.3307 -3.3968
1.2076 -3.3968 0.8448
-0.0001 -0.0003 0.0001
-0.0003 0.0005 -0.0004
0.0001 -0.0004 0.0004

atensor 19 C
-0.0634 -0.2583 0.6293
-0.2583 0.5715 -1.7707
0.6293 -1.7707 4.2999
0.0008 -0.0014 -0.0002
-0.0014 0.0044 0.0005
-0.0002 0.0005 -0.0006

atensor 20 C
0.6619 0.0222 1.8784
0.0222 -0.1551 0.0510
1.8784 0.0510 4.2981
0.0049 0.0001 -0.0005
0.0001 0.0003 -0.0000
-0.0005 -0.0000 -0.0006

atensor 21 H
1.8548 0.1285 3.6045
0.1285 -2.8332 0.0986
3.6045 0.0986 0.8470
0.0006 0.0000 0.0004
0.0000 -0.0002 0.0000
0.0004 0.0000 0.0004

orbtensor 1 Mn
1926.2593 -0.0000 0.0023
-0.0000 1926.2593 -0.0005
0.0023 -0.0005 1937.7318
-2090.6694 -0.0204 0.2167
-0.0204 -2090.7023 -0.1177
0.2167 -0.1177 -116.8214

orbtensor 2 H
25.9439 -5.9353 -0.7778
-5.9353 40.5309 2.1877

-0.7778 2.1877 24.1694
0.6519 6.7675 0.5740
6.7675 -15.9786 -1.6148
0.5740 -1.6148 0.6113

orbtensor 3 C
256.3958 -0.3756 -0.5097
-0.3756 257.3151 1.4313
-0.5097 1.4313 238.7978
-216.1801 20.7711 5.1150
20.7711 -267.2166 -14.3773
5.1150 -14.3773 -80.4711

orbtensor 4 H
42.6271 0.5141 -2.3214
0.5141 23.8484 -0.0635
-2.3214 -0.0635 24.1693
-18.3690 -0.5860 1.7132
-0.5860 3.0416 0.0466
1.7132 0.0466 0.6111

orbtensor 5 C
257.4477 0.0325 -1.5196
0.0325 256.2615 -0.0416
-1.5196 -0.0416 238.7968
-274.5548 -1.7985 15.2603
-1.7985 -208.8426 0.4182
15.2603 0.4182 -80.4728

orbtensor 6 H
25.3397 5.1028 -0.6570
5.1028 41.1372 -2.2269
-0.6570 -2.2269 24.1698
1.3414 -5.8176 0.4844
-5.8176 -16.6691 1.6421
0.4844 1.6421 0.6097

orbtensor 7 C
256.3558 0.3228 -0.4308
0.3228 257.3533 -1.4562
-0.4308 -1.4562 238.7970
-214.0580 -17.8554 4.3194
-17.8554 -269.3255 14.6348
4.3194 14.6348 -80.4592

orbtensor 8 H
36.6285 -8.7711 1.9144
-8.7711 29.8473 -1.3126
1.9144 -1.3126 24.1697
-11.5280 9.9992 -1.4112
9.9992 -3.7974 0.9672
-1.4112 0.9672 0.6097

orbtensor 9 C
257.0690 -0.5540 1.2507
-0.5540 256.6411 -0.8581
1.2507 -0.8581 238.7983
-253.5315 30.6859 -12.5755
30.6859 -229.8157 8.6239
-12.5755 8.6239 -80.4660

orbtensor 10 H
35.6502 9.0890 1.8397
9.0890 30.8257 1.4153
1.8397 1.4153 24.1699
-10.4132 -10.3620 -1.3567
-10.3620 -4.9132 -1.0439

-1.3567 -1.0439 0.6103

orbtensor 11 C

257.0078 0.5740 1.2019
0.5740 256.7037 0.9259
1.2019 0.9259 238.7984
-250.1207 -31.7979 -12.0856
-31.7979 -233.2449 -9.2988
-12.0856 -9.2988 -80.4604

orbtensor 12 H

25.3380 5.1005 0.6564
5.1005 41.1378 2.2285
0.6564 2.2285 24.1701
1.3432 -5.8151 -0.4849
-5.8151 -16.6700 -1.6447
-0.4849 -1.6447 0.6117

orbtensor 13 C

256.3568 0.3218 0.4263
0.3218 257.3548 1.4581
0.4263 1.4581 238.7988
-214.0485 -17.8445 -4.3035
-17.8445 -269.3261 -14.6504
-4.3035 -14.6504 -80.4709

orbtensor 14 H

36.6314 -8.7695 -1.9173
-8.7695 29.8444 1.3137
-1.9173 1.3137 24.1697
-11.5326 9.9986 1.4153
9.9986 -3.7948 -0.9702
1.4153 -0.9702 0.6113

orbtensor 15 C

257.0705 -0.5535 -1.2556
-0.5535 256.6407 0.8604
-1.2556 0.8604 238.7969
-253.5724 30.6840 12.6052
30.6840 -229.8233 -8.6445
12.6052 -8.6445 -80.4723

orbtensor 16 H

35.6475 9.0896 -1.8403
9.0896 30.8285 -1.4156
-1.8403 -1.4156 24.1693
-10.4111 -10.3633 1.3573
-10.3633 -4.9167 1.0443
1.3573 1.0443 0.6101

orbtensor 17 C

257.0072 0.5742 -1.2069
0.5742 256.7028 -0.9242
-1.2069 -0.9242 238.7966
-250.1306 -31.8053 12.1059
-31.8053 -233.2688 9.2928
12.1059 9.2928 -80.4664

orbtensor 18 H

25.9452 -5.9372 0.7766
-5.9372 40.5306 -2.1852
0.7766 -2.1852 24.1692
0.6507 6.7690 -0.5728
6.7690 -15.9776 1.6105
-0.5728 1.6105 0.6099

orbtensor 19 C

256.3932 -0.3745 0.5059
 -0.3745 257.3156 -1.4289
 0.5059 -1.4289 238.7973
 -216.1728 20.7730 -5.0976
 20.7730 -267.2046 14.3526
 -5.0976 14.3526 -80.4610

orbtensor 20 C
 257.4484 0.0320 1.5143
 0.0320 256.2621 0.0437
 1.5143 0.0437 238.7992
 -274.5319 -1.8073 -15.2298
 -1.8073 -208.8323 -0.4326
 -15.2298 -0.4326 -80.4640

orbtensor 21 H
 42.6275 0.5167 2.3191
 0.5167 23.8482 0.0638
 2.3191 0.0638 24.1698
 -18.3680 -0.5892 -1.7100
 -0.5892 3.0416 -0.0472
 -1.7100 -0.0472 0.6109

gtensor (ppt)
 -0.0527 -0.0000 0.0000
 -0.0000 -0.0527 0.0000
 0.0000 0.0000 -0.0797
 0.4186 0.0000 0.0003
 0.0000 0.4186 -0.0000
 0.0003 -0.0000 -0.0915

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-97.3714	497.35243	92615.23790	0.08510	92615.32300	93112.67543
2	H	-0.0456	25.30960	10.76582	0.01884	10.78467	36.09427
3	C	1.6051	62.88030	-1507.88440	0.22654	-1507.65786	-1444.77756
4	H	-0.0457	25.30950	10.80520	0.01890	10.82410	36.13360
5	C	1.6053	62.87860	-1508.00965	0.22668	-1507.78297	-1444.90437
6	H	-0.0445	25.30957	10.51381	0.01885	10.53266	35.84222
7	C	1.6039	62.88780	-1506.75710	0.22644	-1506.53066	-1443.64286
8	H	-0.0436	25.30993	10.30904	0.01876	10.32780	35.63774
9	C	1.6031	62.89840	-1505.97426	0.22617	-1505.74809	-1442.84969
10	H	-0.0444	25.30990	10.48231	0.01875	10.50106	35.81096
11	C	1.6038	62.89463	-1506.60053	0.22621	-1506.37432	-1443.47969
12	H	-0.0439	25.31027	10.37992	0.01882	10.39874	35.70901
13	C	1.6036	62.88830	-1506.41265	0.22634	-1506.18631	-1443.29801
14	H	-0.0455	25.30980	10.75795	0.01890	10.77685	36.08665
15	C	1.6050	62.88003	-1507.72783	0.22666	-1507.50117	-1444.62114
16	H	-0.0462	25.30920	10.90758	0.01888	10.92646	36.23566
17	C	1.6053	62.88027	-1508.00965	0.22662	-1507.78303	-1444.90276
18	H	-0.0448	25.30933	10.59256	0.01877	10.61133	35.92067
19	C	1.6042	62.88923	-1507.00761	0.22630	-1506.78131	-1443.89208
20	C	1.6032	62.89383	-1506.03688	0.22612	-1505.81077	-1442.91694
21	H	-0.0435	25.31000	10.28542	0.01873	10.30415	35.61415
C Average		1.6042	62.88714	-1507.04206	0.22641	-1506.81565	-1443.92851
H Average		-0.0448	25.30971	10.57996	0.01882	10.59878	35.90849

6MnCp2-GTO-BHLYP
 Temperature: 390

Spin: 2.5

atensor 1 Mn

-154.6187 0.0000 0.0005
0.0000 -154.6191 -0.0005
0.0005 -0.0005 -146.2545
-3.3653 0.0000 0.0002
0.0000 -3.3653 -0.0000
0.0002 -0.0000 -3.3388

atensor 2 H

-2.3339 -1.4495 -1.2347
-1.4495 1.2287 3.4733
-1.2347 3.4733 0.8199
0.0008 0.0008 0.0003
0.0008 -0.0010 -0.0008
0.0003 -0.0008 0.0002

atensor 3 C

0.1399 -0.2766 -0.6357
-0.2766 0.8198 1.7882
-0.6357 1.7882 4.0702
-0.0016 -0.0009 0.0002
-0.0009 0.0007 -0.0007
0.0002 -0.0007 -0.0004

atensor 4 H

1.7407 0.1254 -3.6848
0.1254 -2.8450 -0.1006
-3.6848 -0.1006 0.8205
-0.0013 -0.0001 0.0008
-0.0001 0.0011 0.0000
0.0008 0.0000 0.0002

atensor 5 C

0.9161 0.0239 -1.8971
0.0239 0.0408 -0.0517
-1.8971 -0.0517 4.0677
0.0010 0.0001 0.0007
0.0001 -0.0019 0.0000
0.0007 0.0000 -0.0004

atensor 6 H

-2.4809 1.2463 -1.0432
1.2463 1.3771 -3.5362
-1.0432 -3.5362 0.8213
0.0009 -0.0007 0.0002
-0.0007 -0.0011 0.0008
0.0002 0.0008 0.0002

atensor 7 C

0.1113 0.2379 -0.5372
0.2379 0.8474 -1.8202
-0.5372 -1.8202 4.0691
-0.0017 0.0008 0.0002
0.0008 0.0008 0.0007
0.0002 0.0007 -0.0004

atensor 8 H

0.2777 -2.1419 3.0413
-2.1419 -1.3784 -2.0849
3.0413 -2.0849 0.8229
-0.0005 0.0011 -0.0007
0.0011 0.0003 0.0005
-0.0007 0.0005 0.0002

atensor 9 C

0.6357 -0.4088 1.5654
-0.4088 0.3197 -1.0731
1.5654 -1.0731 4.0649
0.0001 -0.0014 -0.0006
-0.0014 -0.0010 0.0004
-0.0006 0.0004 -0.0004

atensor 10 H
0.0381 2.2197 2.9223
2.2197 -1.1398 2.2482
2.9223 2.2482 0.8221
-0.0004 -0.0012 -0.0007
-0.0012 0.0002 -0.0005
-0.0007 -0.0005 0.0002

atensor 11 C
0.5905 0.4237 1.5042
0.4237 0.3658 1.1573
1.5042 1.1573 4.0664
-0.0001 0.0014 -0.0006
0.0014 -0.0008 -0.0004
-0.0006 -0.0004 -0.0004

atensor 12 H
-2.4808 1.2456 1.0426
1.2456 1.3773 3.5368
1.0426 3.5368 0.8226
0.0009 -0.0007 -0.0002
-0.0007 -0.0011 -0.0008
-0.0002 -0.0008 0.0002

atensor 13 C
0.1112 0.2377 0.5366
0.2377 0.8472 1.8201
0.5366 1.8201 4.0686
-0.0017 0.0008 -0.0002
0.0008 0.0008 -0.0007
-0.0002 -0.0007 -0.0004

atensor 14 H
0.2767 -2.1410 -3.0411
-2.1410 -1.3811 2.0834
-3.0411 2.0834 0.8217
-0.0005 0.0011 0.0007
0.0011 0.0003 -0.0005
0.0007 -0.0005 0.0002

atensor 15 C
0.6364 -0.4085 -1.5655
-0.4085 0.3198 1.0721
-1.5655 1.0721 4.0681
0.0001 -0.0014 0.0006
-0.0014 -0.0010 -0.0004
0.0006 -0.0004 -0.0004

atensor 16 H
0.0355 2.2199 -2.9210
2.2199 -1.1407 -2.2480
-2.9210 -2.2480 0.8194
-0.0004 -0.0012 0.0007
-0.0012 0.0002 0.0005
0.0007 0.0005 0.0002

atensor 17 C
0.5915 0.4238 -1.5039
0.4238 0.3672 -1.1576
-1.5039 -1.1576 4.0692

-0.0001 0.0014 0.0006
0.0014 -0.0008 0.0004
0.0006 0.0004 -0.0004

atensor 18 H
-2.3330 -1.4502 1.2349
-1.4502 1.2299 -3.4736
1.2349 -3.4736 0.8198
0.0008 0.0008 -0.0003
0.0008 -0.0010 0.0008
-0.0003 0.0008 0.0002

atensor 19 C
0.1397 -0.2768 0.6357
-0.2768 0.8200 -1.7886
0.6357 -1.7886 4.0687
-0.0016 -0.0009 -0.0002
-0.0009 0.0007 0.0007
-0.0002 0.0007 -0.0004

atensor 20 C
0.9146 0.0238 1.8974
0.0238 0.0392 0.0516
1.8974 0.0516 4.0635
0.0010 0.0001 -0.0007
0.0001 -0.0019 -0.0000
-0.0007 -0.0000 -0.0004

atensor 21 H
1.7436 0.1257 3.6860
0.1257 -2.8426 0.1008
3.6860 0.1008 0.8233
-0.0013 -0.0001 -0.0008
-0.0001 0.0011 -0.0000
-0.0008 -0.0000 0.0002

orbtensor 1 Mn
1923.3811 0.0000 0.0021
0.0000 1923.3811 -0.0007
0.0021 -0.0007 1937.3299
-1260.6081 -0.0057 0.1497
-0.0057 -1260.6179 -0.0717
0.1497 -0.0717 -66.8659

orbtensor 2 H
25.8783 -5.9767 -0.7643
-5.9767 40.5672 2.1495
-0.7643 2.1495 24.0753
0.3403 6.3270 0.4229
6.3270 -15.2075 -1.1892
0.4229 -1.1892 0.3932

orbtensor 3 C
256.4195 -0.3885 -0.5595
-0.3885 257.3709 1.5711
-0.5595 1.5711 238.1745
-210.5887 21.5003 5.1904
21.5003 -263.4261 -14.5911
5.1904 -14.5911 -72.7531

orbtensor 4 H
42.6781 0.5176 -2.2809
0.5176 23.7683 -0.0624
-2.2809 -0.0624 24.0753
-17.4419 -0.5480 1.2621
-0.5480 2.5730 0.0346
1.2621 0.0346 0.3934

orbtensor 5 C
257.5087 0.0334 -1.6678
0.0334 256.2815 -0.0457
-1.6678 -0.0457 238.1737
-271.0188 -1.8626 15.4877
-1.8626 -202.9892 0.4236
15.4877 0.4236 -72.7556

orbtensor 6 H
25.2702 5.1384 -0.6455
5.1384 41.1781 -2.1879
-0.6455 -2.1879 24.0757
0.9846 -5.4389 0.3570
-5.4389 -15.8541 1.2101
0.3570 1.2101 0.3935

orbtensor 7 C
256.3805 0.3339 -0.4727
0.3339 257.4129 -1.5984
-0.4727 -1.5984 238.1745
-208.3951 -18.4844 4.3822
-18.4844 -265.6196 14.8504
4.3822 14.8504 -72.7458

orbtensor 8 H
36.6380 -8.8323 1.8808
-8.8323 29.8094 -1.2896
1.8808 -1.2896 24.0756
-11.0472 9.3501 -1.0397
9.3501 -3.8187 0.7129
-1.0397 0.7129 0.3939

orbtensor 9 C
257.1181 -0.5732 1.3730
-0.5732 256.6750 -0.9419
1.3730 -0.9419 238.1754
-249.2735 31.7705 -12.7606
31.7705 -224.7170 8.7494
-12.7606 8.7494 -72.7531

orbtensor 10 H
35.6527 9.1524 1.8075
9.1524 30.7945 1.3905
1.8075 1.3905 24.0758
-10.0048 -9.6891 -0.9994
-9.6891 -4.8616 -0.7688
-0.9994 -0.7688 0.3936

orbtensor 11 C
257.0539 0.5940 1.3195
0.5940 256.7389 1.0161
1.3195 1.0161 238.1756
-245.7403 -32.9184 -12.2630
-32.9184 -228.2650 -9.4352
-12.2630 -9.4352 -72.7455

orbtensor 12 H
25.2685 5.1361 0.6449
5.1361 41.1785 2.1895
0.6449 2.1895 24.0760
0.9874 -5.4371 -0.3570
-5.4371 -15.8546 -1.2113
-0.3570 -1.2113 0.3936

orbtensor 13 C
256.3799 0.3333 0.4683

0.3333 257.4124 1.6004
0.4683 1.6004 238.1754
-208.3868 -18.4767 -4.3681
-18.4767 -265.6115 -14.8667
-4.3681 -14.8667 -72.7533

orbtensor 14 H
36.6406 -8.8308 -1.8839
-8.8308 29.8063 1.2908
-1.8839 1.2908 24.0756
-11.0512 9.3470 1.0430
9.3470 -3.8176 -0.7145
1.0430 -0.7145 0.3934

orbtensor 15 C
257.1185 -0.5728 -1.3780
-0.5728 256.6743 0.9443
-1.3780 0.9443 238.1740
-249.2964 31.7668 12.7920
31.7668 -224.7115 -8.7745
12.7920 -8.7745 -72.7554

orbtensor 16 H
35.6498 9.1531 -1.8081
9.1531 30.7972 -1.3909
-1.8081 -1.3909 24.0752
-10.0028 -9.6882 1.0003
-9.6882 -4.8665 0.7697
1.0003 0.7697 0.3934

orbtensor 17 C
257.0536 0.5941 -1.3244
0.5941 256.7389 -1.0147
-1.3244 -1.0147 238.1741
-245.7367 -32.9281 12.2856
-32.9281 -228.2835 9.4309
12.2856 9.4309 -72.7519

orbtensor 18 H
25.8800 -5.9787 0.7630
-5.9787 40.5670 -2.1470
0.7630 -2.1470 24.0751
0.3400 6.3291 -0.4217
6.3291 -15.2075 1.1866
-0.4217 1.1866 0.3938

orbtensor 19 C
256.4185 -0.3878 0.5556
-0.3878 257.3725 -1.5685
0.5556 -1.5685 238.1746
-210.5929 21.5083 -5.1741
21.5083 -263.4224 14.5634
-5.1741 14.5634 -72.7473

orbtensor 20 C
257.5097 0.0333 1.6625
0.0333 256.2820 0.0477
1.6625 0.0477 238.1761
-271.0117 -1.8706 -15.4536
-1.8706 -202.9931 -0.4396
-15.4536 -0.4396 -72.7484

orbtensor 21 H
42.6787 0.5203 2.2784
0.5203 23.7684 0.0627
2.2784 0.0627 24.0758
-17.4429 -0.5509 -1.2592

-0.5509 2.5769 -0.0345
-1.2592 -0.0345 0.3939

gtensor (ppt)
-0.0622 0.0000 0.0000
0.0000 -0.0622 0.0000
0.0000 0.0000 -0.0836
-0.8748 -0.0000 0.0002
-0.0000 -0.8748 -0.0000
0.0002 -0.0000 -0.0831

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-155.1872	1065.33340	147543.05811	-0.68223	147542.37588	148607.70928
2	H	-0.0951	25.34893	22.45910	-0.02771	22.43140	47.78033
3	C	1.6762	68.39900	-1573.96357	-0.28828	-1574.25185	-1505.85285
4	H	-0.0946	25.34873	22.34102	-0.02767	22.31335	47.66209
5	C	1.6744	68.40010	-1572.30466	-0.28811	-1572.59277	-1504.19267
6	H	-0.0942	25.34933	22.23869	-0.02772	22.21096	47.56030
7	C	1.6755	68.40247	-1573.30627	-0.28824	-1573.59450	-1505.19204
8	H	-0.0926	25.35033	21.86870	-0.02779	21.84091	47.19124
9	C	1.6730	68.40830	-1570.95875	-0.28816	-1571.24691	-1502.83861
10	H	-0.0932	25.35007	22.01039	-0.02778	21.98261	47.33268
11	C	1.6738	68.40587	-1571.70995	-0.28824	-1571.99820	-1503.59233
12	H	-0.0936	25.34980	22.11273	-0.02778	22.08495	47.43475
13	C	1.6752	68.40537	-1573.05586	-0.28828	-1573.34414	-1504.93877
14	H	-0.0942	25.34903	22.25443	-0.02771	22.22672	47.57576
15	C	1.6743	68.40117	-1572.21076	-0.28819	-1572.49895	-1504.09778
16	H	-0.0953	25.34877	22.49846	-0.02767	22.47080	47.81956
17	C	1.6755	68.39817	-1573.33757	-0.28818	-1573.62575	-1505.22758
18	H	-0.0944	25.34947	22.30166	-0.02772	22.27394	47.62341
19	C	1.6757	68.40100	-1573.49407	-0.28824	-1573.78231	-1505.38131
20	C	1.6720	68.40487	-1570.01974	-0.28814	-1570.30788	-1501.90301
21	H	-0.0919	25.35027	21.70338	-0.02779	21.67559	47.02586
C Average		1.6746	68.40263	-1572.43612	-0.28821	-1572.72433	-1504.32170
H Average		-0.0939	25.34947	22.17886	-0.02773	22.15112	47.50060

6MnCp2-GTO-CAM-B3LYP
Temperature: 390
Spin: 2.5

atensor 2 H
-2.3219 -1.4737 -1.2163
-1.4737 1.3002 3.4215
-1.2163 3.4215 0.8293
0.0002 0.0001 0.0000
0.0001 -0.0001 -0.0001
0.0000 -0.0001 0.0004

atensor 3 C
-0.0869 -0.2652 -0.6342
-0.2652 0.5651 1.7839
-0.6342 1.7839 4.1817
-0.0004 -0.0012 0.0002
-0.0012 0.0026 -0.0006
0.0002 -0.0006 -0.0005

orbtensor 2 H
25.6763 -5.9305 -0.8139

-5.9305 40.2513 2.2893
 -0.8139 2.2893 24.0509
 0.6361 6.5547 0.5497
 6.5547 -15.4717 -1.5471
 0.5497 -1.5471 0.4840

orbtensor 3 C
 255.6674 -0.2506 -0.7075
 -0.2506 256.2794 1.9880
 -0.7075 1.9880 238.3036
 -214.4326 21.4246 5.3568
 21.4246 -267.0770 -15.0559
 5.3568 -15.0559 -76.2538

gtensor (ppt)
 -0.0592 0.0000 0.0000
 0.0000 -0.0592 0.0000
 0.0000 0.0000 -0.0817
 -0.0277 0.0000 0.0002
 0.0000 -0.0277 0.0000
 0.0002 0.0000 -0.0810

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
C Average		1.554	64.1623	-1459.5058	0.0312	-1459.4746	-1395.3123
H Average		-0.064	25.2090	15.1108	0.0027	15.1135	40.3225

6MnCp2-GTO-HF
 Temperature: 390
 Spin: 2.5

atensor 1 Mn
 -278.0583 -0.0006 0.0034
 -0.0006 -278.0558 -0.0008
 0.0034 -0.0008 -262.5742
 -2.2728 -0.0000 0.0002
 -0.0000 -2.2728 -0.0000
 0.0002 -0.0000 -2.0417

atensor 2 H
 -2.3019 -1.3744 -1.2690
 -1.3744 1.0760 3.5697
 -1.2690 3.5697 0.8717
 0.0012 0.0012 0.0005
 0.0012 -0.0018 -0.0013
 0.0005 -0.0013 -0.0001

atensor 3 C
 -0.1653 -0.2926 -0.6300
 -0.2926 0.5537 1.7722
 -0.6300 1.7722 3.0174
 -0.0025 -0.0006 0.0001
 -0.0006 -0.0009 -0.0002
 0.0001 -0.0002 -0.0002

atensor 4 H
 1.5591 0.1190 -3.7870
 0.1190 -2.7907 -0.1034
 -3.7870 -0.1034 0.8690

-0.0023 -0.0001 0.0014
-0.0001 0.0016 0.0000
0.0014 0.0000 -0.0001

atensor 5 C
0.6615 0.0253 -1.8801
0.0253 -0.2640 -0.0512
-1.8801 -0.0512 3.0253
-0.0007 0.0001 0.0002
0.0001 -0.0028 0.0000
0.0002 0.0000 -0.0002

atensor 6 H
-2.4410 1.1817 -1.0721
1.1817 1.2168 -3.6343
-1.0721 -3.6343 0.8733
0.0013 -0.0011 0.0004
-0.0011 -0.0020 0.0013
0.0004 0.0013 -0.0001

atensor 7 C
-0.1958 0.2516 -0.5323
0.2516 0.5826 -1.8040
-0.5323 -1.8040 3.0158
-0.0026 0.0006 0.0000
0.0006 -0.0009 0.0002
0.0000 0.0002 -0.0002

atensor 8 H
0.1731 -2.0313 3.1256
-2.0313 -1.3975 -2.1428
3.1256 -2.1428 0.8734
-0.0010 0.0018 -0.0011
0.0018 0.0004 0.0008
-0.0011 0.0008 -0.0001

atensor 9 C
0.3617 -0.4323 1.5514
-0.4323 0.0274 -1.0636
1.5514 -1.0636 3.0173
-0.0014 -0.0010 -0.0001
-0.0010 -0.0021 0.0001
-0.0001 0.0001 -0.0002

atensor 10 H
-0.0548 2.1052 3.0033
2.1052 -1.1720 2.3105
3.0033 2.3105 0.8717
-0.0008 -0.0019 -0.0011
-0.0019 0.0002 -0.0008
-0.0011 -0.0008 -0.0001

atensor 11 C
0.3149 0.4480 1.4907
0.4480 0.0773 1.1471
1.4907 1.1471 3.0200
-0.0015 0.0010 -0.0001
0.0010 -0.0020 -0.0001
-0.0001 -0.0001 -0.0002

atensor 12 H
-2.4337 1.1803 1.0714
1.1803 1.2217 3.6348
1.0714 3.6348 0.8808
0.0013 -0.0011 -0.0004
-0.0011 -0.0020 -0.0013
-0.0004 -0.0013 -0.0001

atensor 13 C
-0.2056 0.2513 0.5313
0.2513 0.5726 1.8043
0.5313 1.8043 2.9997
-0.0026 0.0006 -0.0000
0.0006 -0.0009 -0.0002
-0.0000 -0.0002 -0.0002

atensor 14 H
0.1737 -2.0301 -3.1253
-2.0301 -1.3985 2.1412
-3.1253 2.1412 0.8738
-0.0010 0.0018 0.0011
0.0018 0.0004 -0.0008
0.0011 -0.0008 -0.0001

atensor 15 C
0.3609 -0.4319 -1.5513
-0.4319 0.0260 1.0631
-1.5513 1.0631 3.0174
-0.0014 -0.0010 0.0001
-0.0010 -0.0021 -0.0001
0.0001 -0.0001 -0.0002

atensor 16 H
-0.0626 2.1070 -3.0020
2.1070 -1.1791 -2.3104
-3.0020 -2.3104 0.8633
-0.0008 -0.0019 0.0011
-0.0019 0.0002 0.0008
0.0011 0.0008 -0.0001

atensor 17 C
0.3265 0.4481 -1.4901
0.4481 0.0892 -1.1474
-1.4901 -1.1474 3.0409
-0.0015 0.0010 0.0001
0.0010 -0.0020 0.0001
0.0001 0.0001 -0.0002

atensor 18 H
-2.2905 -1.3735 1.2691
-1.3735 1.0842 -3.5700
1.2691 -3.5700 0.8805
0.0012 0.0012 -0.0005
0.0012 -0.0018 0.0013
-0.0005 0.0013 -0.0001

atensor 19 C
-0.1807 -0.2927 0.6299
-0.2927 0.5388 -1.7729
0.6299 -1.7729 2.9903
-0.0025 -0.0006 -0.0001
-0.0006 -0.0009 0.0002
-0.0001 0.0002 -0.0002

atensor 20 C
0.6745 0.0252 1.8802
0.0252 -0.2512 0.0510
1.8802 0.0510 3.0462
-0.0007 0.0001 -0.0002
0.0001 -0.0028 -0.0000
-0.0002 -0.0000 -0.0002

atensor 21 H
1.5554 0.1194 3.7883

0.1194 -2.7996 0.1036
3.7883 0.1036 0.8628
-0.0023 -0.0001 -0.0014
-0.0001 0.0016 -0.0000
-0.0014 -0.0000 -0.0001

orbtensor 1 Mn
1920.6367 0.0001 0.0021
0.0001 1920.6362 -0.0009
0.0021 -0.0009 1936.7474
-751.7854 -0.0051 0.1362
-0.0051 -751.7631 -0.0431
0.1362 -0.0431 -24.8763

orbtensor 2 H
26.1690 -6.1299 -0.7618
-6.1299 41.2340 2.1424
-0.7618 2.1424 24.0714
-0.0957 5.9560 0.3158
5.9560 -14.7320 -0.8892
0.3158 -0.8892 0.1583

orbtensor 3 C
258.4227 -0.1060 -0.4427
-0.1060 258.6793 1.2416
-0.4427 1.2416 237.1988
-201.3262 21.7611 5.3006
21.7611 -254.8017 -14.8965
5.3006 -14.8965 -61.2418

orbtensor 4 H
43.3989 0.5308 -2.2734
0.5308 24.0048 -0.0622
-2.2734 -0.0622 24.0714
-16.8360 -0.5160 0.9436
-0.5160 2.0076 0.0260
0.9436 0.0260 0.1584

orbtensor 5 C
258.7164 0.0089 -1.3187
0.0089 258.3832 -0.0362
-1.3187 -0.0362 237.1979
-262.4877 -1.8861 15.8116
-1.8861 -193.6375 0.4324
15.8116 0.4324 -61.2443

orbtensor 6 H
25.5455 5.2701 -0.6434
5.2701 41.8607 -2.1808
-0.6434 -2.1808 24.0719
0.5107 -5.1201 0.2665
-5.1201 -15.3412 0.9047
0.2665 0.9047 0.1586

orbtensor 7 C
258.4125 0.0910 -0.3738
0.0910 258.6928 -1.2632
-0.3738 -1.2632 237.1989
-199.1088 -18.7107 4.4749
-18.7107 -257.0259 15.1611
4.4749 15.1611 -61.2358

orbtensor 8 H
37.2044 -9.0586 1.8746
-9.0586 30.2010 -1.2853
1.8746 -1.2853 24.0718
-10.8160 8.8007 -0.7772

8.8007 -4.0124 0.5326
-0.7772 0.5326 0.1589

orbtensor 9 C
258.6139 -0.1555 1.0845
-0.1555 258.4941 -0.7441
1.0845 -0.7441 237.1995
-240.4728 32.1588 -13.0283
32.1588 -215.6216 8.9339
-13.0283 8.9339 -61.2413

orbtensor 10 H
36.1938 9.3869 1.8015
9.3869 31.2112 1.3859
1.8015 1.3859 24.0719
-9.8349 -9.1197 -0.7472
-9.1197 -4.9939 -0.5744
-0.7472 -0.5744 0.1587

orbtensor 11 C
258.5963 0.1611 1.0422
0.1611 258.5113 0.8027
1.0422 0.8027 237.1999
-236.8980 -33.3187 -12.5202
-33.3187 -219.2140 -9.6337
-12.5202 -9.6337 -61.2345

orbtensor 12 H
25.5435 5.2676 0.6428
5.2676 41.8611 2.1824
0.6428 2.1824 24.0722
0.5122 -5.1179 -0.2673
-5.1179 -15.3408 -0.9053
-0.2673 -0.9053 0.1581

orbtensor 13 C
258.4123 0.0903 0.3692
0.0903 258.6927 1.2652
0.3692 1.2652 237.1995
-199.0893 -18.6992 -4.4590
-18.6992 -257.0133 -15.1797
-4.4590 -15.1797 -61.2412

orbtensor 14 H
37.2069 -9.0569 -1.8778
-9.0569 30.1975 1.2866
-1.8778 1.2866 24.0718
-10.8191 8.7997 0.7798
8.7997 -4.0094 -0.5344
0.7798 -0.5344 0.1578

orbtensor 15 C
258.6120 -0.1554 -1.0899
-0.1554 258.4912 0.7471
-1.0899 0.7471 237.1983
-240.5012 32.1504 13.0608
32.1504 -215.6198 -8.9576
13.0608 -8.9576 -61.2439

orbtensor 16 H
36.1908 9.3875 -1.8022
9.3875 31.2139 -1.3863
-1.8022 -1.3863 24.0714
-9.8324 -9.1210 0.7477
-9.1210 -4.9969 0.5756
0.7477 0.5756 0.1582

orbtensor 17 C
 258.5943 0.1613 -1.0477
 0.1613 258.5092 -0.8012
 -1.0477 -0.8012 237.1985
 -236.9004 -33.3254 12.5432
 -33.3254 -219.2380 9.6276
 12.5432 9.6276 -61.2412

orbtensor 18 H
 26.1708 -6.1318 0.7605
 -6.1318 41.2340 -2.1398
 0.7605 -2.1398 24.0713
 -0.0971 5.9576 -0.3155
 5.9576 -14.7317 0.8866
 -0.3155 0.8866 0.1589

orbtensor 19 C
 258.4225 -0.1051 0.4383
 -0.1051 258.6819 -1.2388
 0.4383 -1.2388 237.1989
 -201.3272 21.7678 -5.2819
 21.7678 -254.8013 14.8699
 -5.2819 14.8699 -61.2360

orbtensor 20 C
 258.7198 0.0087 1.3127
 0.0087 258.3864 0.0384
 1.3127 0.0384 237.2001
 -262.4779 -1.8926 -15.7783
 -1.8926 -193.6302 -0.4488
 -15.7783 -0.4488 -61.2367

orbtensor 21 H
 43.3998 0.5336 2.2709
 0.5336 24.0052 0.0625
 2.2709 0.0625 24.0719
 -16.8357 -0.5185 -0.9409
 -0.5185 2.0069 -0.0257
 -0.9409 -0.0257 0.1587

gtensor (ppt)
 -0.0704 0.0000 0.0000
 0.0000 -0.0704 0.0000
 0.0000 0.0000 -0.0842
 -1.5531 -0.0000 0.0002
 -0.0000 -1.5531 -0.0001
 0.0002 -0.0001 -0.0740

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-275.0919	1416.53183	261482.02783	-2.43039	261479.59744	262896.12927
2	H	-0.1183	25.60167	27.93174	-0.05700	27.87474	53.47641
3	C	1.1341	78.97703	-1064.65459	-0.43139	-1065.08598	-986.10895
4	H	-0.1211	25.60170	28.60071	-0.05699	28.54372	54.14542
5	C	1.1397	78.97600	-1069.94312	-0.43189	-1070.37502	-991.39902
6	H	-0.1172	25.60207	27.67989	-0.05709	27.62280	53.22487
7	C	1.1330	78.97790	-1063.62191	-0.43140	-1064.05331	-985.07541
8	H	-0.1172	25.60257	27.67989	-0.05715	27.62274	53.22531
9	C	1.1342	78.99060	-1064.81105	-0.43156	-1065.24261	-986.25201
10	H	-0.1186	25.60227	28.00257	-0.05709	27.94548	53.54775
11	C	1.1362	78.98700	-1066.62605	-0.43166	-1067.05771	-988.07071

12	H	-0.1107	25.60210	26.12944	-0.05712	26.07232	51.67442
13	C	1.1210	78.98690	-1052.38768	-0.43040	-1052.81809	-973.83119
14	H	-0.1172	25.60183	27.67989	-0.05704	27.62285	53.22468
15	C	1.1335	78.97887	-1064.15390	-0.43148	-1064.58538	-985.60651
16	H	-0.1264	25.60167	29.83635	-0.05700	29.77936	55.38102
17	C	1.1510	78.97413	-1080.52020	-0.43294	-1080.95314	-1001.97901
18	H	-0.1088	25.60207	25.69657	-0.05706	25.63951	51.24158
19	C	1.1149	78.97960	-1046.69234	-0.42976	-1047.12209	-968.14249
20	C	1.1553	78.98717	-1084.55701	-0.43335	-1084.99036	-1006.00319
21	H	-0.1274	25.60227	30.08033	-0.05712	30.02322	55.62548
C Average		1.1353	78.98152	-1065.79679	-0.43158	-1066.22837	-987.24685
H Average		-0.1183	25.60202	27.93174	-0.05706	27.87467	53.47669

=====
6MnCp2-GTO-LC-PBE0
Temperature: 390
Spin: 2.5

atensor 2 H
-2.2909 -1.4349 -1.2290
-1.4349 1.2356 3.4572
-1.2290 3.4572 0.8735
0.0007 0.0006 0.0003
0.0006 -0.0008 -0.0007
0.0003 -0.0007 0.0002

atensor 3 C
-0.2254 -0.2713 -0.6372
-0.2713 0.4415 1.7923
-0.6372 1.7923 3.6652
-0.0010 -0.0011 0.0003
-0.0011 0.0017 -0.0007
0.0003 -0.0007 -0.0004

orbtensor 2 H
25.1700 -6.1982 -0.8981
-6.1982 40.4029 2.5259
-0.8981 2.5259 23.6134
0.6111 6.5195 0.5559
6.5195 -15.4101 -1.5646
0.5559 -1.5646 0.4121

orbtensor 3 C
256.1484 0.0580 -0.7360
0.0580 256.0017 2.0673
-0.7360 2.0673 238.5634
-210.5829 20.3423 5.2708
20.3423 -260.5675 -14.8122
5.2708 -14.8122 -70.1466

gtensor (ppt)
-0.0626 0.0000 0.0000
0.0000 -0.0626 0.0000
0.0000 0.0000 -0.0818
-0.7265 0.0000 0.0002
0.0000 -0.7265 0.0000
0.0002 0.0000 -0.0934

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
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=====

C Average	1.294	69.8055	-1215.0080	-0.2276	-1215.2356	-1145.4301
H Average	-0.061	24.9331	14.3043	-0.0225	14.2818	39.2149

=====
6MnCp2-GTO-PBE0
Temperature: 390
Spin: 2.5

atensor 1 Mn
-136.3156 0.0003 -0.0005
0.0003 -136.3160 -0.0003
-0.0005 -0.0003 -131.8454
-3.6701 0.0000 0.0002
0.0000 -3.6701 0.0000
0.0002 0.0000 -3.9033

atensor 2 H
-2.2780 -1.4416 -1.2187
-1.4416 1.2651 3.4282
-1.2187 3.4282 0.8947
0.0004 0.0003 0.0001
0.0003 -0.0004 -0.0004
0.0001 -0.0004 0.0002

atensor 3 C
-0.0997 -0.2617 -0.6322
-0.2617 0.5435 1.7783
-0.6322 1.7783 3.8701
0.0001 -0.0013 0.0002
-0.0013 0.0032 -0.0006
0.0002 -0.0006 -0.0005

atensor 4 H
1.7763 0.1247 -3.6369
0.1247 -2.7834 -0.0993
-3.6369 -0.0993 0.8979
-0.0005 -0.0000 0.0004
-0.0000 0.0006 0.0000
0.0004 0.0000 0.0002

atensor 5 C
0.6313 0.0226 -1.8866
0.0226 -0.1967 -0.0515
-1.8866 -0.0515 3.8633
0.0036 0.0001 0.0006
0.0001 -0.0004 0.0000
0.0006 0.0000 -0.0005

atensor 6 H
-2.4227 1.2393 -1.0296
1.2393 1.4136 -3.4902
-1.0296 -3.4902 0.8974
0.0005 -0.0003 0.0001
-0.0003 -0.0004 0.0004
0.0001 0.0004 0.0002

atensor 7 C
-0.1286 0.2251 -0.5342
0.2251 0.5678 -1.8102
-0.5342 -1.8102 3.8655
-0.0001 0.0011 0.0002
0.0011 0.0033 0.0006
0.0002 0.0006 -0.0005

atensor 8 H
0.3197 -2.1301 3.0017

-2.1301 -1.3272 -2.0578
3.0017 -2.0578 0.8983
-0.0001 0.0005 -0.0003
0.0005 0.0002 0.0002
-0.0003 0.0002 0.0002

atensor 9 C
0.3687 -0.3867 1.5568
-0.3867 0.0697 -1.0672
1.5568 -1.0672 3.8639
0.0024 -0.0019 -0.0005
-0.0019 0.0009 0.0003
-0.0005 0.0003 -0.0005

atensor 10 H
0.0834 2.2069 2.8843
2.2069 -1.0878 2.2189
2.8843 2.2189 0.8995
-0.0001 -0.0005 -0.0003
-0.0005 0.0002 -0.0002
-0.0003 -0.0002 0.0002

atensor 11 C
0.3229 0.4008 1.4960
0.4008 0.1103 1.1510
1.4960 1.1510 3.8600
0.0021 0.0020 -0.0005
0.0020 0.0011 -0.0004
-0.0005 -0.0004 -0.0005

atensor 12 H
-2.4221 1.2386 1.0290
1.2386 1.4142 3.4908
1.0290 3.4908 0.8992
0.0005 -0.0003 -0.0001
-0.0003 -0.0004 -0.0004
-0.0001 -0.0004 0.0002

atensor 13 C
-0.1294 0.2248 0.5336
0.2248 0.5669 1.8101
0.5336 1.8101 3.8642
-0.0001 0.0011 -0.0002
0.0011 0.0033 -0.0006
-0.0002 -0.0006 -0.0005

atensor 14 H
0.3192 -2.1292 -3.0016
-2.1292 -1.3294 2.0564
-3.0016 2.0564 0.8975
-0.0001 0.0005 0.0003
0.0005 0.0002 -0.0002
0.0003 -0.0002 0.0002

atensor 15 C
0.3690 -0.3864 -1.5568
-0.3864 0.0695 1.0662
-1.5568 1.0662 3.8667
0.0023 -0.0019 0.0005
-0.0019 0.0009 -0.0003
0.0005 -0.0003 -0.0005

atensor 16 H
0.0806 2.2073 -2.8831
2.2073 -1.0889 -2.2188
-2.8831 -2.2188 0.8967
-0.0001 -0.0005 0.0003

-0.0005 0.0002 0.0002
0.0003 0.0002 0.0002

atensor 17 C
0.3245 0.4009 -1.4956
0.4009 0.1123 -1.1512
-1.4956 -1.1512 3.8649
0.0021 0.0019 0.0005
0.0019 0.0011 0.0004
0.0005 0.0004 -0.0005

atensor 18 H
-2.2755 -1.4420 1.2188
-1.4420 1.2674 -3.4285
1.2188 -3.4285 0.8961
0.0004 0.0003 -0.0001
0.0003 -0.0004 0.0004
-0.0001 0.0004 0.0002

atensor 19 C
-0.1016 -0.2618 0.6322
-0.2618 0.5419 -1.7788
0.6322 -1.7788 3.8657
0.0001 -0.0013 -0.0002
-0.0013 0.0032 0.0006
-0.0002 0.0006 -0.0005

atensor 20 C
0.6314 0.0225 1.8870
0.0225 -0.1968 0.0513
1.8870 0.0513 3.8603
0.0037 0.0001 -0.0006
0.0001 -0.0004 -0.0000
-0.0006 -0.0000 -0.0005

atensor 21 H
1.7782 0.1250 3.6381
0.1250 -2.7821 0.0995
3.6381 0.0995 0.8998
-0.0005 -0.0000 -0.0004
-0.0000 0.0006 -0.0000
-0.0004 -0.0000 0.0002

orbtensor 1 Mn
1927.7745 -0.0001 0.0021
-0.0001 1927.7747 -0.0006
0.0021 -0.0006 1938.5494
-1787.1073 -0.0185 0.2062
-0.0185 -1787.1238 -0.0975
0.2062 -0.0975 -101.7413

orbtensor 2 H
25.4794 -6.0670 -0.8611
-6.0670 40.3898 2.4220
-0.8611 2.4220 23.9021
0.6577 6.6278 0.5820
6.6278 -15.6295 -1.6380
0.5820 -1.6380 0.5029

orbtensor 3 C
255.3847 -0.2168 -0.7150
-0.2168 255.9132 2.0084
-0.7150 2.0084 238.7866
-209.8516 19.5804 5.1291
19.5804 -257.9629 -14.4143
5.1291 -14.4143 -75.3012

orbtensor 4 H
42.5324 0.5254 -2.5700
0.5254 23.3374 -0.0703
-2.5700 -0.0703 23.9021
-17.9706 -0.5741 1.7381
-0.5741 2.9982 0.0477
1.7381 0.0477 0.5030

orbtensor 5 C
255.9897 0.0186 -2.1320
0.0186 255.3062 -0.0585
-2.1320 -0.0585 238.7856
-264.8820 -1.6964 15.2999
-1.6964 -202.9347 0.4184
15.2999 0.4184 -75.3041

orbtensor 6 H
24.8619 5.2159 -0.7274
5.2159 41.0095 -2.4655
-0.7274 -2.4655 23.9025
1.3330 -5.6976 0.4914
-5.6976 -16.3064 1.6672
0.4914 1.6672 0.5036

orbtensor 7 C
255.3613 0.1864 -0.6042
0.1864 255.9358 -2.0438
-0.6042 -2.0438 238.7867
-207.8547 -16.8336 4.3310
-16.8336 -259.9587 14.6708
4.3310 14.6708 -75.2944

orbtensor 8 H
36.4009 -8.9656 2.1195
-8.9656 29.4694 -1.4532
2.1195 -1.4532 23.9024
-11.2711 9.7931 -1.4329
9.7931 -3.7000 0.9823
-1.4329 0.9823 0.5038

orbtensor 9 C
255.7720 -0.3192 1.7559
-0.3192 255.5256 -1.2045
1.7559 -1.2045 238.7877
-245.0676 28.9308 -12.6072
28.9308 -222.7092 8.6453
-12.6072 8.6453 -75.3019

orbtensor 10 H
35.4009 9.2905 2.0368
9.2905 30.4695 1.5669
2.0368 1.5669 23.9026
-10.1793 -10.1482 -1.3772
-10.1482 -4.7926 -1.0592
-1.3772 -1.0592 0.5033

orbtensor 11 C
255.7370 0.3307 1.6873
0.3307 255.5622 1.2994
1.6873 1.2994 238.7878
-241.8501 -29.9769 -12.1157
-29.9769 -225.9400 -9.3232
-12.1157 -9.3232 -75.2935

orbtensor 12 H
24.8600 5.2135 0.7268
5.2135 41.0100 2.4671

0.7268 2.4671 23.9030
1.3346 -5.6947 -0.4918
-5.6947 -16.3056 -1.6675
-0.4918 -1.6675 0.5014

orbtensor 13 C
255.3604 0.1852 0.5994
0.1852 255.9356 2.0455
0.5994 2.0455 238.7877
-207.8337 -16.8222 -4.3146
-16.8222 -259.9440 -14.6901
-4.3146 -14.6901 -75.2994

orbtensor 14 H
36.4038 -8.9638 -2.1226
-8.9638 29.4663 1.4543
-2.1226 1.4543 23.9026
-11.2746 9.7916 1.4352
9.7916 -3.6968 -0.9835
1.4352 -0.9835 0.5011

orbtensor 15 C
255.7722 -0.3187 -1.7610
-0.3187 255.5239 1.2065
-1.7610 1.2065 238.7857
-245.0959 28.9251 12.6391
28.9251 -222.7061 -8.6680
12.6391 -8.6680 -75.3010

orbtensor 16 H
35.3983 9.2911 -2.0374
9.2911 30.4723 -1.5673
-2.0374 -1.5673 23.9020
-10.1766 -10.1493 1.3769
-10.1493 -4.7959 1.0599
1.3769 1.0599 0.5013

orbtensor 17 C
255.7367 0.3308 -1.6924
0.3308 255.5610 -1.2979
-1.6924 -1.2979 238.7855
-241.8564 -29.9839 12.1391
-29.9839 -225.9611 9.3173
12.1391 9.3173 -75.2977

orbtensor 18 H
25.4809 -6.0688 0.8599
-6.0688 40.3898 -2.4196
0.8599 -2.4196 23.9020
0.6564 6.6292 -0.5814
6.6292 -15.6285 1.6345
-0.5814 1.6345 0.5018

orbtensor 19 C
255.3828 -0.2156 0.7110
-0.2156 255.9152 -2.0062
0.7110 -2.0062 238.7866
-209.8444 19.5834 -5.1110
19.5834 -257.9555 14.3911
-5.1110 14.3911 -75.2939

orbtensor 20 C
255.9905 0.0183 2.1266
0.0183 255.3068 0.0603
2.1266 0.0603 238.7883
-264.8578 -1.7031 -15.2710
-1.7031 -202.9194 -0.4343

-15.2710 -0.4343 -75.2949

orbtensor 21 H
42.5330 0.5281 2.5677
0.5281 23.3374 0.0706
2.5677 0.0706 23.9026
-17.9689 -0.5769 -1.7347
-0.5769 2.9978 -0.0475
-1.7347 -0.0475 0.5018

gtensor (ppt)
-0.0530 0.0000 0.0000
0.0000 -0.0530 0.0000
0.0000 0.0000 -0.0791
-0.3656 0.0000 0.0003
0.0000 -0.3656 -0.0001
0.0003 -0.0001 -0.1082

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-138.5735	706.04207	131769.97543	-0.10345	131769.87199	132475.91405
2	H	-0.0393	25.10080	9.29065	-0.00844	9.28221	34.38301
3	C	1.4389	68.98960	-1351.36586	-0.08780	-1351.45366	-1282.46406
4	H	-0.0363	25.10083	8.57417	-0.00841	8.56575	33.66659
5	C	1.4335	68.98690	-1346.32566	-0.08769	-1346.41335	-1277.42645
6	H	-0.0371	25.10137	8.77100	-0.00851	8.76250	33.86387
7	C	1.4358	68.99200	-1348.45444	-0.08787	-1348.54231	-1279.55031
8	H	-0.0363	25.10180	8.57417	-0.00859	8.56558	33.66738
9	C	1.4350	69.00220	-1347.73441	-0.08801	-1347.82242	-1278.82022
10	H	-0.0349	25.10147	8.23561	-0.00855	8.22706	33.32853
11	C	1.4320	69.00113	-1344.85430	-0.08791	-1344.94221	-1275.94108
12	H	-0.0361	25.10113	8.53480	-0.00851	8.52629	33.62743
13	C	1.4348	69.00220	-1347.51527	-0.08784	-1347.60312	-1278.60092
14	H	-0.0375	25.10080	8.84974	-0.00842	8.84132	33.94212
15	C	1.4360	68.99293	-1348.61097	-0.08772	-1348.69869	-1279.70576
16	H	-0.0371	25.10047	8.76313	-0.00845	8.75469	33.85515
17	C	1.4348	68.98933	-1347.51527	-0.08777	-1347.60305	-1278.61371
18	H	-0.0373	25.10080	8.80250	-0.00855	8.79395	33.89475
19	C	1.4363	68.99693	-1348.89272	-0.08797	-1348.98069	-1279.98375
20	C	1.4326	69.00450	-1345.41780	-0.08797	-1345.50577	-1276.50127
21	H	-0.0346	25.10123	8.17262	-0.00859	8.16404	33.26527
C Average		1.4350	68.99577	-1347.66867	-0.08785	-1347.75653	-1278.76075
H Average		-0.0366	25.10107	8.65684	-0.00850	8.64834	33.74941

=====
CrL1-STO-B3LYP-No-ZFS
Temperature: 295
Spin: 1.5

atensor 1 N
-1.357 0.233 -0.285
0.233 -2.326 -0.071
-0.285 -0.071 -3.445
-0.011 0.008 0.004
0.000 0.017 0.000
0.005 -0.001 0.025

atensor 2 C
3.003 0.969 0.168
0.969 2.120 -0.041

0.168 -0.041 4.535
-0.035 0.005 0.005
0.023 -0.005 -0.003
0.004 0.000 0.005

atensor 3 C
0.251 0.199 -0.243
0.199 -0.347 -0.068
-0.243 -0.068 -1.530
-0.001 -0.003 0.000
0.001 -0.001 0.000
0.000 0.001 0.002

atensor 4 C
0.506 0.066 0.277
0.066 -0.051 0.086
0.277 0.086 2.619
-0.007 0.002 0.001
0.003 -0.007 0.000
0.001 0.000 0.001

atensor 5 C
-0.360 -0.107 -0.147
-0.107 -0.878 -0.008
-0.147 -0.008 -1.502
-0.002 -0.002 0.001
0.001 0.004 0.000
0.001 0.000 0.003

atensor 6 C
1.246 -0.551 -0.089
-0.551 -0.861 0.116
-0.089 0.116 0.427
0.004 0.002 0.000
-0.021 -0.011 0.003
0.001 0.000 0.003

atensor 7 C
0.247 -0.112 0.054
-0.112 -0.033 0.038
0.054 0.038 0.621
-0.001 0.002 0.000
-0.002 -0.003 0.000
0.000 0.000 0.001

atensor 8 C
-0.148 -0.162 -0.091
-0.162 -0.225 -0.002
-0.091 -0.002 -0.880
0.000 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 9 C
-1.017 -0.252 0.090
-0.252 -0.874 0.050
0.090 0.050 -0.405
-0.006 -0.006 0.001
0.004 0.005 -0.001
0.001 0.001 0.001

atensor 10 C
1.296 -1.005 -0.199
-1.005 1.058 0.076
-0.199 0.076 -0.482
-0.003 0.005 0.001
0.006 -0.006 0.000

0.001 0.000 0.006

atensor 11 C
-0.212 -1.669 0.010
-1.669 -2.468 0.280
0.010 0.281 -0.593
0.074 0.027 0.001
-0.016 -0.021 0.006
0.003 0.000 0.090

atensor 12 C
0.162 -0.510 0.008
-0.510 2.274 -2.277
0.008 -2.277 1.396
0.074 -0.002 0.003
0.005 -0.001 0.055
-0.004 0.037 0.058

atensor 13 C
1.837 1.600 -0.870
1.600 -0.031 -1.040
-0.870 -1.040 1.047
0.046 -0.020 0.003
-0.037 0.012 0.028
0.006 0.026 0.074

atensor 14 C
0.237 0.089 0.272
0.089 2.590 2.249
0.272 2.249 1.008
0.073 -0.011 -0.006
-0.009 -0.007 -0.050
0.001 -0.031 0.065

atensor 15 C
-0.169 -0.224 0.291
-0.224 0.325 -0.808
0.291 -0.808 0.901
0.011 0.001 -0.005
-0.001 0.001 0.005
-0.004 0.008 -0.001

atensor 16 H
-0.299 -0.160 0.193
-0.159 1.194 -1.451
0.193 -1.451 1.076
0.004 0.003 -0.004
-0.001 -0.001 0.007
0.000 0.011 -0.002

atensor 17 H
-0.253 -1.272 1.579
-1.272 -0.081 -1.801
1.579 -1.801 0.715
0.004 0.008 -0.011
0.003 0.000 0.010
-0.012 0.017 -0.005

atensor 18 H
-1.864 -0.239 0.531
-0.239 -1.121 -1.861
0.531 -1.861 3.086
0.009 -0.002 -0.009
-0.004 0.010 0.006
-0.002 0.019 -0.026

atensor 19 C

0.523 0.439 -0.628
0.439 0.062 -0.387
-0.628 -0.387 0.408
0.004 -0.004 0.005
-0.003 0.003 0.000
0.008 0.003 0.005

atensor 20 H
-0.746 0.966 -0.884
0.966 -0.709 -0.889
-0.884 -0.889 -0.864
0.003 -0.005 0.002
-0.003 0.003 0.003
0.005 0.006 0.002

atensor 21 H
-0.337 0.814 -2.376
0.814 -1.732 -1.049
-2.376 -1.049 1.135
0.003 -0.006 0.011
0.000 0.012 -0.002
0.019 0.012 -0.011

atensor 22 H
1.634 1.138 -1.493
1.138 -1.150 -0.555
-1.493 -0.555 -0.793
-0.004 -0.009 0.008
-0.002 0.008 0.001
0.012 0.005 0.007

atensor 23 C
0.816 0.563 0.479
0.563 0.107 0.266
0.479 0.266 0.069
0.001 -0.005 -0.004
-0.004 0.003 0.001
-0.007 -0.002 0.008

atensor 24 C
-0.242 -0.016 0.004
-0.016 0.442 0.875
0.004 0.875 0.860
0.013 -0.001 0.002
-0.002 0.000 -0.005
0.001 -0.008 -0.001

atensor 25 H
-0.306 0.212 0.144
0.212 1.397 1.425
0.144 1.425 0.891
0.004 0.001 0.002
-0.002 -0.002 -0.006
-0.002 -0.012 -0.001

atensor 26 H
-1.806 0.287 0.725
0.287 -0.844 2.129
0.725 2.129 2.756
0.010 -0.007 0.001
-0.005 0.008 -0.007
-0.007 -0.020 -0.025

atensor 27 H
-0.956 -0.856 -1.100
-0.856 0.189 2.141
-1.100 2.141 1.147

0.009 0.004 0.007
0.002 -0.002 -0.011
0.009 -0.019 -0.008

atensor 28 H
1.326 0.635 -0.210
0.635 0.383 -0.100
-0.210 -0.100 -0.086
-0.001 -0.005 0.001
-0.001 0.001 0.000
0.001 0.001 0.005

atensor 29 H
0.266 0.216 -0.193
0.216 -1.622 -0.012
-0.193 -0.012 -1.136
-0.005 -0.002 0.001
0.002 0.001 0.000
0.001 0.000 0.003

atensor 30 C
2.181 1.864 0.432
1.864 0.080 0.642
0.432 0.642 0.585
0.047 -0.025 0.006
-0.042 0.009 -0.013
0.004 -0.015 0.077

atensor 31 H
2.191 1.315 0.611
1.315 -1.095 0.234
0.611 0.234 -1.404
-0.008 -0.011 -0.003
-0.003 0.008 0.000
-0.008 -0.003 0.011

atensor 32 H
0.910 1.240 2.345
1.240 -1.597 0.927
2.345 0.927 -0.253
-0.005 -0.010 -0.012
-0.001 0.011 0.000
-0.021 -0.011 -0.002

atensor 33 H
-0.343 1.211 0.655
1.211 -0.613 0.574
0.655 0.574 -1.378
0.001 -0.006 -0.002
-0.004 0.002 -0.002
-0.004 -0.005 0.005

atensor 34 H
-0.709 3.399 -0.496
3.399 1.156 -0.608
-0.496 -0.608 -3.530
0.010 -0.016 0.003
-0.013 -0.005 0.003
0.003 0.003 0.031

atensor 35 H
0.260 -0.268 -0.105
-0.267 -0.614 0.035
-0.105 0.035 -0.607
-0.003 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.002

atensor 36 H
0.394 -0.340 -0.060
-0.340 0.187 0.032
-0.060 0.032 -0.155
-0.002 0.003 0.000
0.002 -0.001 0.000
0.000 0.000 0.002

atensor 37 H
-0.448 -0.660 -0.013
-0.659 0.608 0.040
-0.013 0.040 -0.721
-0.001 0.005 0.001
0.004 -0.004 0.000
0.001 0.000 0.004

orbtensor 1 N
-474.253 42.621 54.646
42.621 -554.445 12.292
54.646 12.292 -49.420
321.908 -3.095 -4.195
-3.095 333.325 -1.146
-4.195 -1.146 289.376

orbtensor 2 C
-290.380 29.718 25.812
29.718 -327.217 4.616
25.812 4.616 -86.732
259.734 6.157 -4.502
6.157 262.009 -2.027
-4.502 -2.027 227.389

orbtensor 3 C
-235.460 -43.230 25.844
-43.230 -281.787 13.732
25.844 13.732 -52.301
258.227 -1.272 -5.050
-1.272 255.091 -1.090
-5.050 -1.090 219.716

orbtensor 4 C
-312.723 -24.872 33.785
-24.872 -252.344 9.958
33.785 9.958 -64.246
253.049 3.208 -4.118
3.208 263.224 -1.845
-4.118 -1.845 222.808

orbtensor 5 C
-297.587 2.497 32.442
2.497 -277.437 7.715
32.442 7.715 -51.135
271.049 1.356 -5.507
1.356 260.856 -1.286
-5.507 -1.286 229.771

orbtensor 6 C
-291.233 13.539 23.492
13.539 -319.586 5.584
23.492 5.584 -110.666
270.148 0.775 -4.948
0.775 269.095 -1.381
-4.948 -1.381 232.943

orbtensor 7 C
-303.739 15.108 30.835

15.108	-224.768	3.695
30.835	3.695	-66.668
254.972	-5.023	-4.247
-5.023	260.993	-0.745
-4.247	-0.745	221.494

orbtensor 8 C

-261.865	47.707	25.416
47.707	-279.944	1.678
25.416	1.678	-56.717
259.432	2.439	-4.691
2.439	257.449	-1.485
-4.691	-1.485	224.612

orbtensor 9 C

-251.259	-36.814	26.424
-36.814	-295.528	13.020
26.424	13.020	-61.318
259.363	-5.600	-4.967
-5.600	254.864	-0.501
-4.967	-0.501	220.262

orbtensor 10 C

-310.160	-19.099	30.379
-19.099	-253.327	8.387
30.379	8.387	-85.726
267.907	1.836	-5.073
1.836	262.635	-1.399
-5.073	-1.399	230.014

orbtensor 11 C

-235.482	31.014	0.225
31.014	-122.998	-7.678
0.225	-7.678	-225.095
258.494	-3.659	-0.589
-3.659	231.099	1.225
-0.589	1.225	253.013

orbtensor 12 C

-218.148	25.217	0.271
25.217	-106.855	24.615
0.271	24.615	-248.338
262.713	-4.331	-4.697
-4.331	237.430	-2.123
-4.697	-2.123	256.369

orbtensor 13 C

-249.933	3.145	10.907
3.145	-94.906	12.207
10.907	12.207	-241.482
261.219	-1.260	3.582
-1.260	236.023	-1.169
3.582	-1.169	260.345

orbtensor 14 C

-220.509	16.600	-8.564
16.600	-111.175	-39.527
-8.564	-39.527	-241.492
264.677	-3.230	2.722
-3.230	237.876	4.303
2.722	4.303	253.963

orbtensor 15 C

-53.864	2.373	4.306
2.373	-46.136	3.313
4.306	3.313	-50.413
218.616	-1.250	4.415

-1.250	215.876	-4.018
4.415	-4.018	229.300

orbtensor 16 H

3.249	-0.793	-0.234
-0.793	2.475	1.619
-0.234	1.619	1.380
23.793	1.058	-0.412
1.058	29.015	-6.751
-0.412	-6.751	29.583

orbtensor 17 H

2.273	0.487	-2.684
0.487	3.395	2.394
-2.684	2.394	2.122
31.637	-0.734	0.907
-0.734	21.183	-2.118
0.907	-2.118	29.698

orbtensor 18 H

5.338	0.447	-0.574
0.447	4.180	1.642
-0.574	1.642	-2.647
21.908	-2.651	-0.298
-2.651	26.160	2.103
-0.298	2.103	31.441

orbtensor 19 C

-51.063	-1.775	-3.470
-1.775	-42.257	2.334
-3.470	2.334	-53.244
225.023	1.432	-8.690
1.432	215.094	-0.316
-8.690	-0.316	222.303

orbtensor 20 H

2.766	-0.751	1.448
-0.751	2.732	0.923
1.448	0.923	2.624
26.738	3.410	-4.328
3.410	28.571	-4.958
-4.328	-4.958	26.819

orbtensor 21 H

2.484	-1.436	3.565
-1.436	4.670	0.384
3.565	0.384	-0.786
26.072	2.564	-3.211
2.564	24.627	3.826
-3.211	3.826	29.573

orbtensor 22 H

-1.840	-0.839	2.014
-0.839	3.088	0.914
2.014	0.914	3.736
34.639	-2.113	-1.036
-2.113	22.624	-0.809
-1.036	-0.809	26.254

orbtensor 23 C

-49.460	-2.146	2.633
-2.146	-42.521	-2.533
2.633	-2.533	-54.520
229.104	2.048	6.768
2.048	215.137	0.207
6.768	0.207	218.182

orbtensor 24 C
-55.800 1.187 -2.926
1.187 -46.690 -3.907
-2.926 -3.907 -47.989
217.141 -0.258 -1.231
-0.258 216.505 5.160
-1.231 5.160 230.147

orbtensor 25 H
3.248 -1.191 -0.154
-1.191 2.213 -1.402
-0.154 -1.402 1.574
24.320 2.809 1.541
2.809 29.915 6.213
1.541 6.213 28.156

orbtensor 26 H
5.090 -0.071 -1.443
-0.071 3.865 -2.160
-1.443 -2.160 -2.148
22.739 -2.946 2.830
-2.946 25.939 -1.013
2.830 -1.013 30.837

orbtensor 27 H
3.566 0.007 2.324
0.007 2.997 -2.568
2.324 -2.568 1.149
31.066 -0.162 -1.278
-0.162 21.521 2.816
-1.278 2.816 29.928

orbtensor 28 H
-4.606 -6.768 0.638
-6.768 -15.745 1.372
0.638 1.372 -1.680
31.151 5.344 -1.374
5.344 40.813 -1.349
-1.374 -1.349 22.231

orbtensor 29 H
-19.017 -3.447 2.272
-3.447 -2.771 0.450
2.272 0.450 -2.732
41.784 2.871 -2.726
2.871 30.313 -0.678
-2.726 -0.678 21.950

orbtensor 30 C
-254.742 -1.972 -7.183
-1.972 -97.399 -22.204
-7.183 -22.204 -234.310
259.411 -0.940 -3.291
-0.940 236.317 3.172
-3.291 3.172 261.853

orbtensor 31 H
-2.445 -1.119 -0.289
-1.119 2.925 -0.561
-0.289 -0.561 4.448
34.638 -1.806 -1.058
-1.806 22.786 1.546
-1.058 1.546 26.096

orbtensor 32 H
0.519 -1.796 -3.793
-1.796 4.616 -0.267

```

-3.793   -0.267   1.203
27.855   1.780   3.583
1.780   24.088  -4.073
3.583   -4.073   28.328

```

```

orbtensor 33 H
2.052   -1.040  -1.211
-1.040   2.576  -0.646
-1.211   -0.646   3.438
28.796   4.806   3.435
4.806   29.166   3.656
3.435   3.656   24.165

```

```

orbtensor 34 H
-7.004   5.777   0.668
5.777  -14.295  -0.269
0.668   -0.269  -0.312
34.028  -3.157  -1.828
-3.157  36.236  -0.186
-1.828  -0.186  19.344

```

```

orbtensor 35 H
-19.030   0.775   2.128
0.775   -2.676  -0.087
2.128   -0.087  -2.703
42.762  -0.734  -2.697
-0.734  30.198  -0.198
-2.697  -0.198  22.152

```

```

orbtensor 36 H
-7.351   8.082   0.340
8.082  -13.546  -0.669
0.340   -0.669  -2.611
33.609  -6.811  -1.212
-6.811  38.412   0.327
-1.212   0.327  22.592

```

```

orbtensor 37 H
-4.483  -6.078   0.650
-6.078  -16.555   1.328
0.650   1.328  -1.172
31.241   2.358  -1.385
2.358  40.373  -0.973
-1.385  -0.973  21.424

```

```

gtensor (ppt)
-0.163   0.005   0.000
0.005  -0.150  -0.001
0.000  -0.001  -0.163
-8.989   4.226  -1.119
4.226  -6.414  -0.897
-1.119  -0.897  -16.302

```

```

averaging
2H Average:34
4H Average:29
9,10H Average:16,17,18,20,21,22
5H Average:35
8,11H Average:25,26,27,31,32,33
6H Average:36
3H Average:28
7H Average:37

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
---	----	------------	---------------	-----------	-----------	--------------	---------

1	N	-2.3657	-44.50300	4313.25299	-3.24041	4310.01259	4265.50959
2	C	3.2077	14.93433	-1680.90507	0.40018	-1680.50488	-1665.57055
3	C	-0.5420	54.49533	284.02282	-0.88173	283.14109	337.63642
4	C	1.0203	36.58933	-534.68257	1.28806	-533.39451	-496.80518
5	C	-0.9117	45.17233	477.73827	-0.33540	477.40287	522.57520
6	C	0.2693	16.90033	-141.13803	0.77924	-140.35879	-123.45846
7	C	0.2773	47.42800	-145.33025	0.39190	-144.93835	-97.51035
8	C	-0.4177	47.65567	218.86876	-0.23883	218.62992	266.28559
9	C	-0.7653	42.12800	401.05560	0.46880	401.52440	443.65240
10	C	0.6230	37.11433	-326.46904	-0.08736	-326.55640	-289.44207
11	C	-1.0433	53.01033	546.73520	1.95633	548.69153	601.70187
12	C	1.3210	61.05700	-692.24013	-0.10335	-692.34348	-631.28648
13	C	0.9950	57.08867	-521.40721	-1.18480	-522.59202	-465.50335
14	C	1.3220	61.11333	-692.76416	-0.10378	-692.86794	-631.75461
15	C	0.3560	171.12633	-186.55374	0.45196	-186.10178	-14.97544
16	H	0.6573	29.83167	-86.63317	0.01852	-86.61465	-56.78298
17	H	0.1267	30.10267	-16.69402	0.34893	-16.34509	13.75757
18	H	0.0313	28.79333	-4.12957	0.55166	-3.57791	25.21542
19	C	0.3350	171.95200	-175.54916	-0.39462	-175.94378	-3.99178
20	H	-0.7703	30.08333	101.52599	-0.27654	101.24946	131.33279
21	H	-0.3100	28.88000	40.85641	0.00252	40.85894	69.73894
22	H	-0.0993	29.50033	13.09163	-0.35772	12.73391	42.23424
23	C	0.3347	171.97400	-175.37449	-0.39401	-175.76850	-3.79450
24	C	0.3573	171.10467	-187.25244	0.45342	-186.79902	-15.69435
25	H	0.6610	29.80867	-87.11642	0.01877	-87.09765	-57.28899
26	H	0.0330	28.77400	-4.34923	0.55184	-3.79739	24.97661
27	H	0.1263	30.07567	-16.65009	0.34943	-16.30066	13.77501
28	H	0.5427	24.05467	-71.52069	-0.22378	-71.74447	-47.68980
29	H	-0.8310	23.17567	109.52155	-0.05389	109.46766	132.64333
30	C	0.9930	57.04333	-520.35916	-1.18096	-521.54012	-464.49678
31	H	-0.0990	29.48267	13.04769	-0.35739	12.69031	42.17297
32	H	-0.3120	28.86967	41.12000	0.00295	41.12296	69.99262
33	H	-0.7753	30.06433	102.18497	-0.27612	101.90885	131.97319
34	H	-1.0157	22.66567	133.85967	-1.20434	132.65533	155.32100
35	H	-0.3207	23.56767	42.26223	0.01688	42.27910	65.84677
36	H	0.1417	23.70167	-18.67094	0.01124	-18.65970	5.04196
37	H	-0.1873	23.60933	24.68958	-0.00736	24.68221	48.29154
38	Cr	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
39	Cl	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
40	Cl	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000

=====
CrL1-STO-B3LYP-ORCA

Temperature: 295

Spin: 1.5

atensor 1 N

-1.357 0.233 -0.285
0.233 -2.326 -0.071
-0.285 -0.071 -3.445
-0.011 0.008 0.004
0.000 0.017 0.000
0.005 -0.001 0.025

atensor 2 C

3.003 0.969 0.168
0.969 2.120 -0.041
0.168 -0.041 4.535
-0.035 0.005 0.005
0.023 -0.005 -0.003
0.004 0.000 0.005

atensor 3 C

0.251 0.199 -0.243
0.199 -0.347 -0.068
-0.243 -0.068 -1.530

-0.001 -0.003 0.000
0.001 -0.001 0.000
0.000 0.001 0.002

atensor 4 C
0.506 0.066 0.277
0.066 -0.051 0.086
0.277 0.086 2.619
-0.007 0.002 0.001
0.003 -0.007 0.000
0.001 0.000 0.001

atensor 5 C
-0.360 -0.107 -0.147
-0.107 -0.878 -0.008
-0.147 -0.008 -1.502
-0.002 -0.002 0.001
0.001 0.004 0.000
0.001 0.000 0.003

atensor 6 C
1.246 -0.551 -0.089
-0.551 -0.861 0.116
-0.089 0.116 0.427
0.004 0.002 0.000
-0.021 -0.011 0.003
0.001 0.000 0.003

atensor 7 C
0.247 -0.112 0.054
-0.112 -0.033 0.038
0.054 0.038 0.621
-0.001 0.002 0.000
-0.002 -0.003 0.000
0.000 0.000 0.001

atensor 8 C
-0.148 -0.162 -0.091
-0.162 -0.225 -0.002
-0.091 -0.002 -0.880
0.000 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 9 C
-1.017 -0.252 0.090
-0.252 -0.874 0.050
0.090 0.050 -0.405
-0.006 -0.006 0.001
0.004 0.005 -0.001
0.001 0.001 0.001

atensor 10 C
1.296 -1.005 -0.199
-1.005 1.058 0.076
-0.199 0.076 -0.482
-0.003 0.005 0.001
0.006 -0.006 0.000
0.001 0.000 0.006

atensor 11 C
-0.212 -1.669 0.010
-1.669 -2.468 0.280
0.010 0.281 -0.593
0.074 0.027 0.001
-0.016 -0.021 0.006
0.003 0.000 0.090

atensor 12 C
0.162 -0.510 0.008
-0.510 2.274 -2.277
0.008 -2.277 1.396
0.074 -0.002 0.003
0.005 -0.001 0.055
-0.004 0.037 0.058

atensor 13 C
1.837 1.600 -0.870
1.600 -0.031 -1.040
-0.870 -1.040 1.047
0.046 -0.020 0.003
-0.037 0.012 0.028
0.006 0.026 0.074

atensor 14 C
0.237 0.089 0.272
0.089 2.590 2.249
0.272 2.249 1.008
0.073 -0.011 -0.006
-0.009 -0.007 -0.050
0.001 -0.031 0.065

atensor 15 C
-0.169 -0.224 0.291
-0.224 0.325 -0.808
0.291 -0.808 0.901
0.011 0.001 -0.005
-0.001 0.001 0.005
-0.004 0.008 -0.001

atensor 16 H
-0.299 -0.160 0.193
-0.159 1.194 -1.451
0.193 -1.451 1.076
0.004 0.003 -0.004
-0.001 -0.001 0.007
0.000 0.011 -0.002

atensor 17 H
-0.253 -1.272 1.579
-1.272 -0.081 -1.801
1.579 -1.801 0.715
0.004 0.008 -0.011
0.003 0.000 0.010
-0.012 0.017 -0.005

atensor 18 H
-1.864 -0.239 0.531
-0.239 -1.121 -1.861
0.531 -1.861 3.086
0.009 -0.002 -0.009
-0.004 0.010 0.006
-0.002 0.019 -0.026

atensor 19 C
0.523 0.439 -0.628
0.439 0.062 -0.387
-0.628 -0.387 0.408
0.004 -0.004 0.005
-0.003 0.003 0.000
0.008 0.003 0.005

atensor 20 H
-0.746 0.966 -0.884

0.966 -0.709 -0.889
-0.884 -0.889 -0.864
0.003 -0.005 0.002
-0.003 0.003 0.003
0.005 0.006 0.002

atensor 21 H
-0.337 0.814 -2.376
0.814 -1.732 -1.049
-2.376 -1.049 1.135
0.003 -0.006 0.011
0.000 0.012 -0.002
0.019 0.012 -0.011

atensor 22 H
1.634 1.138 -1.493
1.138 -1.150 -0.555
-1.493 -0.555 -0.793
-0.004 -0.009 0.008
-0.002 0.008 0.001
0.012 0.005 0.007

atensor 23 C
0.816 0.563 0.479
0.563 0.107 0.266
0.479 0.266 0.069
0.001 -0.005 -0.004
-0.004 0.003 0.001
-0.007 -0.002 0.008

atensor 24 C
-0.242 -0.016 0.004
-0.016 0.442 0.875
0.004 0.875 0.860
0.013 -0.001 0.002
-0.002 0.000 -0.005
0.001 -0.008 -0.001

atensor 25 H
-0.306 0.212 0.144
0.212 1.397 1.425
0.144 1.425 0.891
0.004 0.001 0.002
-0.002 -0.002 -0.006
-0.002 -0.012 -0.001

atensor 26 H
-1.806 0.287 0.725
0.287 -0.844 2.129
0.725 2.129 2.756
0.010 -0.007 0.001
-0.005 0.008 -0.007
-0.007 -0.020 -0.025

atensor 27 H
-0.956 -0.856 -1.100
-0.856 0.189 2.141
-1.100 2.141 1.147
0.009 0.004 0.007
0.002 -0.002 -0.011
0.009 -0.019 -0.008

atensor 28 H
1.326 0.635 -0.210
0.635 0.383 -0.100
-0.210 -0.100 -0.086
-0.001 -0.005 0.001

-0.001 0.001 0.000
0.001 0.001 0.005

atensor 29 H
0.266 0.216 -0.193
0.216 -1.622 -0.012
-0.193 -0.012 -1.136
-0.005 -0.002 0.001
0.002 0.001 0.000
0.001 0.000 0.003

atensor 30 C
2.181 1.864 0.432
1.864 0.080 0.642
0.432 0.642 0.585
0.047 -0.025 0.006
-0.042 0.009 -0.013
0.004 -0.015 0.077

atensor 31 H
2.191 1.315 0.611
1.315 -1.095 0.234
0.611 0.234 -1.404
-0.008 -0.011 -0.003
-0.003 0.008 0.000
-0.008 -0.003 0.011

atensor 32 H
0.910 1.240 2.345
1.240 -1.597 0.927
2.345 0.927 -0.253
-0.005 -0.010 -0.012
-0.001 0.011 0.000
-0.021 -0.011 -0.002

atensor 33 H
-0.343 1.211 0.655
1.211 -0.613 0.574
0.655 0.574 -1.378
0.001 -0.006 -0.002
-0.004 0.002 -0.002
-0.004 -0.005 0.005

atensor 34 H
-0.709 3.399 -0.496
3.399 1.156 -0.608
-0.496 -0.608 -3.530
0.010 -0.016 0.003
-0.013 -0.005 0.003
0.003 0.003 0.031

atensor 35 H
0.260 -0.268 -0.105
-0.267 -0.614 0.035
-0.105 0.035 -0.607
-0.003 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.002

atensor 36 H
0.394 -0.340 -0.060
-0.340 0.187 0.032
-0.060 0.032 -0.155
-0.002 0.003 0.000
0.002 -0.001 0.000
0.000 0.000 0.002

atensor 37 H
-0.448 -0.660 -0.013
-0.659 0.608 0.040
-0.013 0.040 -0.721
-0.001 0.005 0.001
0.004 -0.004 0.000
0.001 0.000 0.004

orbtensor 1 N
-474.253 42.621 54.646
42.621 -554.445 12.292
54.646 12.292 -49.420
321.908 -3.095 -4.195
-3.095 333.325 -1.146
-4.195 -1.146 289.376

orbtensor 2 C
-290.380 29.718 25.812
29.718 -327.217 4.616
25.812 4.616 -86.732
259.734 6.157 -4.502
6.157 262.009 -2.027
-4.502 -2.027 227.389

orbtensor 3 C
-235.460 -43.230 25.844
-43.230 -281.787 13.732
25.844 13.732 -52.301
258.227 -1.272 -5.050
-1.272 255.091 -1.090
-5.050 -1.090 219.716

orbtensor 4 C
-312.723 -24.872 33.785
-24.872 -252.344 9.958
33.785 9.958 -64.246
253.049 3.208 -4.118
3.208 263.224 -1.845
-4.118 -1.845 222.808

orbtensor 5 C
-297.587 2.497 32.442
2.497 -277.437 7.715
32.442 7.715 -51.135
271.049 1.356 -5.507
1.356 260.856 -1.286
-5.507 -1.286 229.771

orbtensor 6 C
-291.233 13.539 23.492
13.539 -319.586 5.584
23.492 5.584 -110.666
270.148 0.775 -4.948
0.775 269.095 -1.381
-4.948 -1.381 232.943

orbtensor 7 C
-303.739 15.108 30.835
15.108 -224.768 3.695
30.835 3.695 -66.668
254.972 -5.023 -4.247
-5.023 260.993 -0.745
-4.247 -0.745 221.494

orbtensor 8 C
-261.865 47.707 25.416
47.707 -279.944 1.678

25.416	1.678	-56.717
259.432	2.439	-4.691
2.439	257.449	-1.485
-4.691	-1.485	224.612

orbtensor 9 C

-251.259	-36.814	26.424
-36.814	-295.528	13.020
26.424	13.020	-61.318
259.363	-5.600	-4.967
-5.600	254.864	-0.501
-4.967	-0.501	220.262

orbtensor 10 C

-310.160	-19.099	30.379
-19.099	-253.327	8.387
30.379	8.387	-85.726
267.907	1.836	-5.073
1.836	262.635	-1.399
-5.073	-1.399	230.014

orbtensor 11 C

-235.482	31.014	0.225
31.014	-122.998	-7.678
0.225	-7.678	-225.095
258.494	-3.659	-0.589
-3.659	231.099	1.225
-0.589	1.225	253.013

orbtensor 12 C

-218.148	25.217	0.271
25.217	-106.855	24.615
0.271	24.615	-248.338
262.713	-4.331	-4.697
-4.331	237.430	-2.123
-4.697	-2.123	256.369

orbtensor 13 C

-249.933	3.145	10.907
3.145	-94.906	12.207
10.907	12.207	-241.482
261.219	-1.260	3.582
-1.260	236.023	-1.169
3.582	-1.169	260.345

orbtensor 14 C

-220.509	16.600	-8.564
16.600	-111.175	-39.527
-8.564	-39.527	-241.492
264.677	-3.230	2.722
-3.230	237.876	4.303
2.722	4.303	253.963

orbtensor 15 C

-53.864	2.373	4.306
2.373	-46.136	3.313
4.306	3.313	-50.413
218.616	-1.250	4.415
-1.250	215.876	-4.018
4.415	-4.018	229.300

orbtensor 16 H

3.249	-0.793	-0.234
-0.793	2.475	1.619
-0.234	1.619	1.380
23.793	1.058	-0.412
1.058	29.015	-6.751

-0.412 -6.751 29.583

orbtensor 17 H

2.273 0.487 -2.684
0.487 3.395 2.394
-2.684 2.394 2.122
31.637 -0.734 0.907
-0.734 21.183 -2.118
0.907 -2.118 29.698

orbtensor 18 H

5.338 0.447 -0.574
0.447 4.180 1.642
-0.574 1.642 -2.647
21.908 -2.651 -0.298
-2.651 26.160 2.103
-0.298 2.103 31.441

orbtensor 19 C

-51.063 -1.775 -3.470
-1.775 -42.257 2.334
-3.470 2.334 -53.244
225.023 1.432 -8.690
1.432 215.094 -0.316
-8.690 -0.316 222.303

orbtensor 20 H

2.766 -0.751 1.448
-0.751 2.732 0.923
1.448 0.923 2.624
26.738 3.410 -4.328
3.410 28.571 -4.958
-4.328 -4.958 26.819

orbtensor 21 H

2.484 -1.436 3.565
-1.436 4.670 0.384
3.565 0.384 -0.786
26.072 2.564 -3.211
2.564 24.627 3.826
-3.211 3.826 29.573

orbtensor 22 H

-1.840 -0.839 2.014
-0.839 3.088 0.914
2.014 0.914 3.736
34.639 -2.113 -1.036
-2.113 22.624 -0.809
-1.036 -0.809 26.254

orbtensor 23 C

-49.460 -2.146 2.633
-2.146 -42.521 -2.533
2.633 -2.533 -54.520
229.104 2.048 6.768
2.048 215.137 0.207
6.768 0.207 218.182

orbtensor 24 C

-55.800 1.187 -2.926
1.187 -46.690 -3.907
-2.926 -3.907 -47.989
217.141 -0.258 -1.231
-0.258 216.505 5.160
-1.231 5.160 230.147

orbtensor 25 H

3.248	-1.191	-0.154
-1.191	2.213	-1.402
-0.154	-1.402	1.574
24.320	2.809	1.541
2.809	29.915	6.213
1.541	6.213	28.156

orbtensor 26 H

5.090	-0.071	-1.443
-0.071	3.865	-2.160
-1.443	-2.160	-2.148
22.739	-2.946	2.830
-2.946	25.939	-1.013
2.830	-1.013	30.837

orbtensor 27 H

3.566	0.007	2.324
0.007	2.997	-2.568
2.324	-2.568	1.149
31.066	-0.162	-1.278
-0.162	21.521	2.816
-1.278	2.816	29.928

orbtensor 28 H

-4.606	-6.768	0.638
-6.768	-15.745	1.372
0.638	1.372	-1.680
31.151	5.344	-1.374
5.344	40.813	-1.349
-1.374	-1.349	22.231

orbtensor 29 H

-19.017	-3.447	2.272
-3.447	-2.771	0.450
2.272	0.450	-2.732
41.784	2.871	-2.726
2.871	30.313	-0.678
-2.726	-0.678	21.950

orbtensor 30 C

-254.742	-1.972	-7.183
-1.972	-97.399	-22.204
-7.183	-22.204	-234.310
259.411	-0.940	-3.291
-0.940	236.317	3.172
-3.291	3.172	261.853

orbtensor 31 H

-2.445	-1.119	-0.289
-1.119	2.925	-0.561
-0.289	-0.561	4.448
34.638	-1.806	-1.058
-1.806	22.786	1.546
-1.058	1.546	26.096

orbtensor 32 H

0.519	-1.796	-3.793
-1.796	4.616	-0.267
-3.793	-0.267	1.203
27.855	1.780	3.583
1.780	24.088	-4.073
3.583	-4.073	28.328

orbtensor 33 H

2.052	-1.040	-1.211
-1.040	2.576	-0.646
-1.211	-0.646	3.438

```

28.796    4.806    3.435
4.806    29.166    3.656
3.435    3.656    24.165

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orbtensor 34 H
-7.004    5.777    0.668
5.777   -14.295   -0.269
0.668    -0.269   -0.312
34.028   -3.157   -1.828
-3.157   36.236   -0.186
-1.828   -0.186   19.344

```

```

orbtensor 35 H
-19.030    0.775    2.128
0.775   -2.676   -0.087
2.128   -0.087   -2.703
42.762   -0.734   -2.697
-0.734   30.198   -0.198
-2.697   -0.198   22.152

```

```

orbtensor 36 H
-7.351    8.082    0.340
8.082   -13.546   -0.669
0.340   -0.669   -2.611
33.609   -6.811   -1.212
-6.811   38.412    0.327
-1.212    0.327   22.592

```

```

orbtensor 37 H
-4.483   -6.078    0.650
-6.078  -16.555    1.328
0.650    1.328   -1.172
31.241    2.358   -1.385
2.358   40.373   -0.973
-1.385   -0.973   21.424

```

```

gtensor (ppt)
-0.163    0.005    0.000
0.005   -0.150   -0.001
0.000   -0.001   -0.163
-8.989    4.226   -1.119
4.226   -6.414   -0.897
-1.119   -0.897  -16.302

```

```

zfstensor (cm-1)
-1.014174    0.341954   -0.001144
 0.341954    0.575629   -0.090077
-0.001144   -0.090077   -0.949768

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.3657	-44.50300	4313.21407	-2.54608	4310.66799	4266.16499
2	C	3.2077	14.93433	-1680.88990	-0.58253	-1681.47243	-1666.53810
3	C	-0.5420	54.49533	284.02026	-0.48423	283.53604	338.03137
4	C	1.0203	36.58933	-534.67775	-0.31234	-534.99009	-498.40076
5	C	-0.9117	45.17233	477.73396	-0.38653	477.34742	522.51976
6	C	0.2693	16.90033	-141.13676	-1.45978	-142.59654	-125.69621
7	C	0.2773	47.42800	-145.32894	-0.17499	-145.50393	-98.07593
8	C	-0.4177	47.65567	218.86678	-0.07108	218.79571	266.45137
9	C	-0.7653	42.12800	401.05198	0.14073	401.19271	443.32071
10	C	0.6230	37.11433	-326.46609	-0.17626	-326.64235	-289.52802
11	C	-1.0433	53.01033	546.73027	-1.54418	545.18609	598.19642
12	C	1.3210	61.05700	-692.23388	1.49424	-690.73964	-629.68264
13	C	0.9950	57.08867	-521.40251	-1.53273	-522.93523	-465.84657
14	C	1.3220	61.11333	-692.75791	1.56268	-691.19523	-630.08189

15	C	0.3560	171.12633	-186.55205	0.43004	-186.12201	-14.99568
16	H	0.6573	29.83167	-86.63239	0.28107	-86.35132	-56.51965
17	H	0.1267	30.10267	-16.69387	0.13468	-16.55919	13.54348
18	H	0.0313	28.79333	-4.12954	0.18160	-3.94793	24.84540
19	C	0.3350	171.95200	-175.54758	-0.45052	-175.99810	-4.04610
20	H	-0.7703	30.08333	101.52508	-0.04293	101.48215	131.56548
21	H	-0.3100	28.88000	40.85605	-0.35425	40.50180	69.38180
22	H	-0.0993	29.50033	13.09151	-0.56792	12.52359	42.02392
23	C	0.3347	171.97400	-175.37290	-0.43494	-175.80784	-3.83384
24	C	0.3573	171.10467	-187.25075	0.45233	-186.79842	-15.69376
25	H	0.6610	29.80867	-87.11563	0.29188	-86.82375	-57.01509
26	H	0.0330	28.77400	-4.34919	0.19612	-4.15307	24.62093
27	H	0.1263	30.07567	-16.64994	0.14487	-16.50506	13.57060
28	H	0.5427	24.05467	-71.52005	-0.18347	-71.70351	-47.64885
29	H	-0.8310	23.17567	109.52056	-0.34076	109.17980	132.35546
30	C	0.9930	57.04333	-520.35446	-1.50462	-521.85909	-464.81575
31	H	-0.0990	29.48267	13.04758	-0.56206	12.48552	41.96819
32	H	-0.3120	28.86967	41.11963	-0.34049	40.77915	69.64881
33	H	-0.7753	30.06433	102.18405	-0.03547	102.14857	132.21291
34	H	-1.0157	22.66567	133.85846	0.25138	134.10984	156.77551
35	H	-0.3207	23.56767	42.26185	-0.15485	42.10700	65.67467
36	H	0.1417	23.70167	-18.67077	-0.03607	-18.70685	4.99482
37	H	-0.1873	23.60933	24.68935	0.18834	24.87770	48.48703
38	Cr	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
39	Cl	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
40	Cl	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000

=====
CrL1-STO-BHLYP-No-ZFS

Temperature: 295

Spin: 1.5

atensor 1 N

-2.125 0.224 -0.335
0.224 -3.099 -0.083
-0.335 -0.083 -4.593
-0.012 -0.005 0.006
0.000 0.023 0.000
0.006 0.001 0.030

atensor 2 C

3.423 0.966 0.143
0.966 2.477 -0.045
0.143 -0.045 4.763
-0.030 0.000 0.005
0.021 -0.009 -0.002
0.004 0.001 0.007

atensor 3 C

-0.286 0.201 -0.320
0.201 -0.849 -0.090
-0.320 -0.090 -2.649
-0.002 -0.002 0.001
0.000 0.001 0.000
0.001 0.000 0.003

atensor 4 C

1.034 0.074 0.284
0.074 0.467 0.087
0.284 0.087 3.202
-0.008 0.001 0.001
0.003 -0.005 0.000
0.001 0.000 0.001

atensor 5 C

-0.733 -0.119 -0.227

-0.119 -1.263 -0.028
-0.227 -0.028 -2.478
-0.003 0.000 0.001
0.001 0.004 0.000
0.001 0.000 0.004

atensor 6 C
1.568 -0.566 -0.042
-0.566 -0.571 0.132
-0.042 0.132 1.101
-0.003 0.005 0.001
-0.018 -0.008 0.003
0.002 0.000 0.006

atensor 7 C
0.643 -0.112 0.132
-0.112 0.331 0.060
0.132 0.060 1.609
-0.003 0.002 0.000
-0.001 -0.003 0.000
0.001 0.000 0.001

atensor 8 C
-0.488 -0.156 -0.176
-0.156 -0.560 -0.026
-0.176 -0.026 -1.859
0.000 0.002 0.000
0.001 0.001 0.000
0.000 0.000 0.001

atensor 9 C
-0.675 -0.243 0.152
-0.243 -0.539 0.066
0.152 0.066 0.411
-0.006 -0.003 0.001
0.006 0.003 -0.001
0.001 0.000 0.001

atensor 10 C
1.182 -1.044 -0.286
-1.044 0.966 0.057
-0.286 0.057 -1.265
-0.004 0.010 0.001
0.008 -0.004 -0.001
0.001 -0.001 0.009

atensor 11 C
-0.859 -1.742 0.007
-1.742 -3.282 0.294
0.007 0.294 -1.279
0.091 0.036 0.000
-0.018 -0.032 0.007
0.002 0.000 0.100

atensor 12 C
-0.125 -0.594 0.046
-0.594 1.966 -2.215
0.046 -2.215 1.180
0.091 -0.002 0.006
0.009 -0.005 0.070
0.000 0.049 0.073

atensor 13 C
1.492 1.625 -0.903
1.625 -0.552 -1.003
-0.903 -1.003 0.670
0.053 -0.029 0.003

-0.045 0.011 0.033
0.009 0.034 0.084

atensor 14 C
-0.062 -0.008 0.263
-0.008 2.277 2.217
0.263 2.217 0.812
0.088 -0.014 -0.008
-0.009 -0.013 -0.065
-0.003 -0.041 0.083

atensor 15 C
-0.255 -0.228 0.292
-0.228 0.261 -0.816
0.292 -0.816 0.799
0.013 0.001 -0.007
0.000 0.001 0.007
-0.005 0.011 -0.002

atensor 16 H
-0.506 -0.171 0.190
-0.171 0.995 -1.472
0.190 -1.472 0.883
0.007 0.004 -0.005
0.000 -0.002 0.011
-0.001 0.017 -0.004

atensor 17 H
-0.310 -1.300 1.608
-1.300 -0.124 -1.831
1.608 -1.831 0.680
0.005 0.013 -0.017
0.007 0.001 0.015
-0.019 0.025 -0.008

atensor 18 H
-1.896 -0.241 0.541
-0.241 -1.196 -1.889
0.541 -1.889 3.148
0.016 -0.002 -0.012
-0.004 0.014 0.011
-0.004 0.027 -0.038

atensor 19 C
0.579 0.450 -0.633
0.450 0.125 -0.394
-0.633 -0.394 0.450
0.003 -0.006 0.007
-0.004 0.004 0.001
0.010 0.005 0.005

atensor 20 H
-0.879 0.984 -0.891
0.984 -0.842 -0.910
-0.891 -0.910 -0.992
0.003 -0.008 0.005
-0.006 0.004 0.005
0.009 0.010 0.003

atensor 21 H
-0.371 0.810 -2.417
0.810 -1.830 -1.064
-2.417 -1.064 1.147
0.004 -0.009 0.019
-0.001 0.016 0.000
0.030 0.017 -0.017

atensor 22 H
1.623 1.159 -1.521
1.159 -1.212 -0.566
-1.521 -0.566 -0.834
-0.010 -0.014 0.013
-0.004 0.012 0.002
0.018 0.008 0.010

atensor 23 C
0.874 0.576 0.479
0.576 0.172 0.269
0.479 0.269 0.110
0.000 -0.007 -0.005
-0.005 0.004 0.001
-0.008 -0.003 0.009

atensor 24 C
-0.331 -0.018 0.000
-0.018 0.378 0.880
0.000 0.880 0.757
0.015 -0.001 0.002
-0.002 -0.001 -0.007
0.001 -0.011 -0.003

atensor 25 H
-0.509 0.207 0.150
0.207 1.201 1.447
0.150 1.448 0.692
0.008 0.000 0.002
-0.003 -0.004 -0.011
-0.002 -0.018 -0.003

atensor 26 H
-1.837 0.293 0.738
0.293 -0.913 2.166
0.738 2.166 2.813
0.016 -0.009 -0.001
-0.007 0.011 -0.013
-0.010 -0.029 -0.036

atensor 27 H
-1.025 -0.876 -1.118
-0.876 0.150 2.178
-1.118 2.178 1.120
0.013 0.007 0.012
0.004 -0.002 -0.018
0.014 -0.028 -0.013

atensor 28 H
1.657 0.553 -0.218
0.553 0.557 -0.087
-0.218 -0.087 0.162
-0.004 -0.007 0.002
-0.003 0.002 0.001
0.002 0.001 0.008

atensor 29 H
0.105 0.234 -0.194
0.234 -1.808 -0.014
-0.194 -0.014 -1.300
-0.007 -0.002 0.002
0.002 0.003 0.000
0.002 0.000 0.005

atensor 30 C
1.849 1.882 0.452
1.882 -0.448 0.610

0.452 0.610 0.196
0.053 -0.036 0.008
-0.052 0.008 -0.015
0.003 -0.021 0.088

atensor 31 H
2.191 1.340 0.627
1.340 -1.156 0.240
0.627 0.240 -1.458
-0.016 -0.016 -0.005
-0.005 0.012 0.000
-0.011 -0.004 0.017

atensor 32 H
0.898 1.243 2.392
1.243 -1.693 0.949
2.392 0.949 -0.267
-0.009 -0.015 -0.020
-0.003 0.015 -0.001
-0.031 -0.015 -0.002

atensor 33 H
-0.473 1.235 0.660
1.235 -0.743 0.589
0.660 0.589 -1.511
0.000 -0.011 -0.004
-0.008 0.003 -0.004
-0.007 -0.007 0.007

atensor 34 H
-0.865 3.518 -0.510
3.518 1.095 -0.629
-0.510 -0.629 -3.759
0.009 -0.033 0.006
-0.023 -0.007 0.005
0.005 0.006 0.042

atensor 35 H
0.099 -0.250 -0.115
-0.250 -0.987 0.037
-0.115 0.037 -0.839
-0.005 0.002 0.001
0.002 0.001 0.000
0.001 0.000 0.004

atensor 36 H
0.723 -0.235 -0.073
-0.235 0.444 0.019
-0.073 0.019 0.107
-0.003 0.004 0.001
0.003 -0.001 0.000
0.001 0.000 0.003

atensor 37 H
-0.757 -0.609 -0.003
-0.609 0.416 0.032
-0.003 0.032 -0.946
-0.001 0.008 0.001
0.006 -0.006 0.000
0.001 -0.001 0.007

atensor 38 Cr
30.601 3.477 -0.392
3.477 40.592 -0.868
-0.392 -0.868 28.577
3.930 -0.623 0.148
-0.679 2.801 0.161

0.150 0.154 4.881

atensor 39 C1
5.893 0.342 1.317
0.342 2.820 -4.294
1.317 -4.294 -3.518
0.459 0.030 0.039
-0.001 0.205 -0.124
0.015 -0.289 0.259

atensor 40 C1
4.602 1.203 -3.594
1.203 3.364 3.655
-3.594 3.655 -2.774
0.432 0.099 -0.093
0.029 0.233 0.123
-0.065 0.275 0.259

orbtensor 1 N
-478.421 37.800 58.006
37.800 -529.028 12.750
58.006 12.750 -29.102
320.744 -4.183 -3.987
-4.183 334.554 -1.042
-3.987 -1.042 289.493

orbtensor 2 C
-292.975 32.052 27.309
32.052 -332.570 4.835
27.309 4.835 -77.390
258.152 6.195 -4.410
6.195 262.226 -2.070
-4.410 -2.070 226.518

orbtensor 3 C
-229.836 -46.014 26.614
-46.014 -277.394 14.315
26.614 14.315 -41.595
255.842 -0.895 -5.272
-0.895 253.738 -1.231
-5.272 -1.231 215.759

orbtensor 4 C
-317.413 -29.314 35.628
-29.314 -253.117 10.855
35.628 10.855 -56.379
251.601 3.779 -4.169
3.779 262.605 -1.956
-4.169 -1.956 221.137

orbtensor 5 C
-295.581 2.264 33.339
2.264 -275.138 7.979
33.339 7.979 -42.188
272.067 1.917 -5.793
1.917 258.902 -1.326
-5.793 -1.326 228.777

orbtensor 6 C
-292.153 14.945 25.230
14.945 -324.705 6.027
25.230 6.027 -98.220
269.754 0.621 -4.861
0.621 269.659 -1.373
-4.861 -1.373 233.161

orbtensor 7 C

-305.851	18.660	32.016
18.660	-221.023	3.369
32.016	3.369	-59.096
254.058	-5.895	-4.280
-5.895	260.351	-0.659
-4.280	-0.659	220.090

orbtensor 8 C

-260.113	49.604	25.991
49.604	-276.393	1.521
25.991	1.521	-50.084
258.434	3.078	-4.701
3.078	257.517	-1.602
-4.701	-1.602	223.716

orbtensor 9 C

-251.091	-39.939	27.779
-39.939	-293.682	13.686
27.779	13.686	-51.594
258.164	-5.429	-5.255
-5.429	252.581	-0.561
-5.255	-0.561	216.925

orbtensor 10 C

-310.633	-22.422	31.751
-22.422	-245.558	8.861
31.751	8.861	-76.892
268.499	2.770	-5.340
2.770	261.156	-1.511
-5.340	-1.511	228.841

orbtensor 11 C

-230.852	34.773	1.022
34.773	-113.263	-8.102
1.022	-8.102	-213.293
258.457	-2.889	-0.375
-2.889	229.154	1.255
-0.375	1.255	254.801

orbtensor 12 C

-209.785	26.600	0.540
26.600	-99.860	28.452
0.540	28.452	-238.823
264.787	-4.145	-5.487
-4.145	237.688	-1.551
-5.487	-1.551	256.094

orbtensor 13 C

-247.839	1.930	11.754
1.930	-86.222	14.085
11.754	14.085	-236.640
261.878	-1.720	5.225
-1.720	236.035	-1.009
5.225	-1.009	260.725

orbtensor 14 C

-212.167	16.984	-8.496
16.984	-104.683	-43.376
-8.496	-43.376	-231.383
266.986	-3.170	2.833
-3.170	238.051	3.657
2.833	3.657	253.536

orbtensor 15 C

-43.168	2.306	2.594
2.306	-36.536	4.185
2.594	4.185	-42.804

215.199	-1.373	4.957
-1.373	212.112	-4.262
4.957	-4.262	226.871

orbtensor 16 H

3.443	-0.603	-0.438
-0.603	3.075	1.373
-0.438	1.373	1.707
23.626	1.004	-0.318
1.004	28.541	-6.508
-0.318	-6.508	29.322

orbtensor 17 H

3.260	0.569	-2.985
0.569	3.308	2.641
-2.985	2.641	2.216
31.045	-0.746	0.857
-0.746	21.019	-2.089
0.857	-2.089	29.597

orbtensor 18 H

5.756	0.177	-0.914
0.177	4.833	2.388
-0.914	2.388	-2.608
21.653	-2.585	-0.196
-2.585	25.798	1.833
-0.196	1.833	31.053

orbtensor 19 C

-41.914	-2.139	-1.803
-2.139	-32.689	2.609
-1.803	2.609	-44.249
221.944	1.392	-9.219
1.392	211.213	-0.282
-9.219	-0.282	219.217

orbtensor 20 H

3.034	-0.657	1.313
-0.657	3.411	0.669
1.313	0.669	2.916
26.520	3.261	-4.213
3.261	28.117	-4.741
-4.213	-4.741	26.546

orbtensor 21 H

2.773	-1.483	3.955
-1.483	5.222	0.951
3.955	0.951	-0.401
25.867	2.576	-3.261
2.576	24.290	3.579
-3.261	3.579	29.100

orbtensor 22 H

-1.274	-1.299	2.413
-1.299	3.008	0.909
2.413	0.909	3.912
34.228	-1.920	-1.153
-1.920	22.679	-0.769
-1.153	-0.769	26.220

orbtensor 23 C

-41.128	-2.685	1.177
-2.685	-32.992	-2.687
1.177	-2.687	-44.669
226.284	2.041	7.229
2.041	211.253	0.225
7.229	0.225	214.833

orbtensor 24 C
-44.449 0.954 -2.171
0.954 -37.229 -4.901
-2.171 -4.901 -40.902
213.521 -0.328 -1.458
-0.328 212.784 5.527
-1.458 5.527 227.879

orbtensor 25 H
3.542 -0.938 0.040
-0.938 2.835 -1.227
0.040 -1.227 1.766
24.102 2.690 1.445
2.690 29.410 6.011
1.445 6.011 27.976

orbtensor 26 H
5.661 -0.506 -1.204
-0.506 4.407 -2.862
-1.204 -2.862 -2.161
22.422 -2.821 2.697
-2.821 25.612 -0.770
2.697 -0.770 30.475

orbtensor 27 H
4.639 0.038 2.367
0.038 2.867 -2.820
2.367 -2.820 1.187
30.531 -0.173 -1.113
-0.173 21.354 2.793
-1.113 2.793 29.774

orbtensor 28 H
-4.720 -6.622 0.621
-6.622 -15.396 1.338
0.621 1.338 -1.844
31.124 5.238 -1.379
5.238 40.783 -1.338
-1.379 -1.338 22.138

orbtensor 29 H
-18.999 -3.568 2.204
-3.568 -2.751 0.443
2.204 0.443 -3.249
41.577 2.890 -2.696
2.890 30.270 -0.678
-2.696 -0.678 21.972

orbtensor 30 C
-252.860 -3.702 -7.127
-3.702 -88.938 -23.940
-7.127 -23.940 -229.015
259.249 -1.527 -4.754
-1.527 236.318 3.203
-4.754 3.203 263.062

orbtensor 31 H
-2.089 -1.582 -0.702
-1.582 2.861 -0.407
-0.702 -0.407 4.827
34.306 -1.619 -0.874
-1.619 22.831 1.449
-0.874 1.449 25.991

orbtensor 32 H
0.622 -2.016 -4.091

-2.016	5.089	-0.803
-4.091	-0.803	1.847
27.656	1.854	3.554
1.854	23.783	-3.849
3.554	-3.849	27.816

orbtensor 33 H

2.383	-0.876	-1.098
-0.876	3.276	-0.450
-1.098	-0.450	3.632
28.520	4.600	3.336
4.600	28.685	3.502
3.336	3.502	23.974

orbtensor 34 H

-6.658	5.700	0.671
5.700	-13.888	-0.259
0.671	-0.259	0.042
33.766	-3.339	-1.802
-3.339	35.943	-0.156
-1.802	-0.156	19.225

orbtensor 35 H

-18.943	1.012	2.024
1.012	-2.882	-0.129
2.024	-0.129	-3.335
42.730	-0.875	-2.654
-0.875	30.412	-0.178
-2.654	-0.178	22.407

orbtensor 36 H

-7.272	7.824	0.308
7.824	-13.384	-0.647
0.308	-0.647	-2.836
33.497	-6.652	-1.196
-6.652	38.506	0.305
-1.196	0.305	22.643

orbtensor 37 H

-4.379	-6.099	0.625
-6.099	-16.042	1.306
0.625	1.306	-1.231
31.016	2.404	-1.403
2.404	39.908	-0.975
-1.403	-0.975	21.071

orbtensor 38 Cr

-6004.070	853.540	-165.268
853.540	-4214.931	-208.875
-165.268	-208.875	-7020.271
1805.955	2.281	-0.386
2.281	1813.332	-0.632
-0.386	-0.632	1803.663

orbtensor 39 Cl

-11.457	-11.543	26.108
-11.543	-151.844	0.994
26.108	0.994	-121.979
1141.748	-0.588	-2.081
-0.588	1145.692	4.904
-2.081	4.904	1146.300

orbtensor 40 Cl

-31.253	-13.605	-49.201
-13.605	-151.432	4.906
-49.201	4.906	-102.257
1143.105	-1.638	3.092

-1.638 1145.041 -4.571
 3.092 -4.571 1145.592

gtensor (ppt)

-0.169 0.006 0.000
 0.006 -0.155 -0.001
 0.000 -0.001 -0.170
 -16.478 5.017 -1.296
 5.017 -12.327 -1.095
 -1.296 -1.095 -24.914

averaging

2H Average:34
 4H Average:29
 9,10H Average:16,17,18,20,21,22
 5H Average:35
 8,11H Average:25,26,27,31,32,33
 6H Average:36
 3H Average:28
 7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.2587	-30.58667	5919.52554	-4.58483	5914.94071	5884.35404
2	C	3.5437	14.65367	-1850.13064	0.46479	-1849.66585	-1835.01219
3	C	-1.2607	58.83800	658.18776	-1.44191	656.74585	715.58385
4	C	1.5637	36.14467	-816.38255	1.63006	-814.75248	-778.60782
5	C	-1.4897	48.94633	777.74752	-0.76500	776.98252	825.92885
6	C	0.6977	19.16533	-364.24828	1.29015	-362.95813	-343.79279
7	C	0.8593	49.50967	-448.65364	0.88947	-447.76416	-398.25450
8	C	-0.9683	51.02567	505.56199	-0.71674	504.84525	555.87091
9	C	-0.2683	43.76767	140.09549	0.86137	140.95686	184.72453
10	C	0.2947	41.80433	-153.84399	-0.53332	-154.37732	-112.57298
11	C	-1.7537	61.66800	915.58060	2.58119	918.16179	979.82979
12	C	1.0600	70.03367	-553.42070	-0.06929	-553.48999	-483.45632
13	C	0.5860	62.64567	-305.94767	-1.25349	-307.20116	-244.55549
14	C	1.0617	70.11333	-554.29086	-0.07078	-554.36164	-484.24831
15	C	0.2723	177.22467	-142.18387	0.50234	-141.68153	35.54313
16	H	0.4577	29.90467	-60.09570	0.00687	-60.08883	-30.18416
17	H	0.0813	30.14833	-10.67979	0.41791	-10.26188	19.88645
18	H	0.0160	28.82833	-2.10094	0.68001	-1.42093	27.40740
19	C	0.3887	177.84067	-202.92092	-0.46529	-203.38621	-25.54555
20	H	-0.9010	30.18133	118.30931	-0.33285	117.97646	148.15779
21	H	-0.3503	28.95033	46.00188	0.04376	46.04564	74.99597
22	H	-0.1370	29.59100	17.98932	-0.39824	17.59108	47.18208
23	C	0.3897	177.86033	-203.44302	-0.46552	-203.90854	-26.04821
24	C	0.2717	177.20133	-141.83581	0.50341	-141.33239	35.86894
25	H	0.4617	29.87700	-60.62094	0.00708	-60.61386	-30.73686
26	H	0.0180	28.80533	-2.36356	0.68044	-1.68312	27.12221
27	H	0.0810	30.11733	-10.63602	0.41871	-10.21731	19.90003
28	H	0.7940	24.02833	-104.25926	-0.23249	-104.49175	-80.46341
29	H	-1.0007	22.94000	131.39643	-0.04439	131.35204	154.29204
30	C	0.5820	62.60533	-303.85929	-1.24882	-305.10811	-242.50278
31	H	-0.1367	29.57567	17.94555	-0.39792	17.54763	47.12330
32	H	-0.3527	28.93767	46.30827	0.04469	46.35295	75.29062
33	H	-0.9057	30.15667	118.92209	-0.33251	118.58958	148.74624
34	H	-1.1617	22.81000	152.53716	-1.51463	151.02253	173.83253
35	H	-0.5757	23.46300	75.59015	0.03966	75.62981	99.09281
36	H	0.4243	23.71800	-55.71874	-0.01211	-55.73085	-32.01285
37	H	-0.4290	23.44767	56.33151	-0.03719	56.29433	79.74200
38	Cr	37.1273	-3938.77400	86076.28563	34.12989	86110.41552	82171.64152
39	Cl	2.0393	1049.48667	-2729.89161	-13.21591	-2743.10752	-1693.62085
40	Cl	2.0387	1049.59867	-2728.99920	-13.20248	-2742.20168	-1692.60301

=====
CrL1-STO-BHLYP-ORCA
Temperature: 295
Spin: 1.5

atensor 1 N
-2.125 0.224 -0.335
0.224 -3.099 -0.083
-0.335 -0.083 -4.593
-0.012 -0.005 0.006
0.000 0.023 0.000
0.006 0.001 0.030

atensor 2 C
3.423 0.966 0.143
0.966 2.477 -0.045
0.143 -0.045 4.763
-0.030 0.000 0.005
0.021 -0.009 -0.002
0.004 0.001 0.007

atensor 3 C
-0.286 0.201 -0.320
0.201 -0.849 -0.090
-0.320 -0.090 -2.649
-0.002 -0.002 0.001
0.000 0.001 0.000
0.001 0.000 0.003

atensor 4 C
1.034 0.074 0.284
0.074 0.467 0.087
0.284 0.087 3.202
-0.008 0.001 0.001
0.003 -0.005 0.000
0.001 0.000 0.001

atensor 5 C
-0.733 -0.119 -0.227
-0.119 -1.263 -0.028
-0.227 -0.028 -2.478
-0.003 0.000 0.001
0.001 0.004 0.000
0.001 0.000 0.004

atensor 6 C
1.568 -0.566 -0.042
-0.566 -0.571 0.132
-0.042 0.132 1.101
-0.003 0.005 0.001
-0.018 -0.008 0.003
0.002 0.000 0.006

atensor 7 C
0.643 -0.112 0.132
-0.112 0.331 0.060
0.132 0.060 1.609
-0.003 0.002 0.000
-0.001 -0.003 0.000
0.001 0.000 0.001

atensor 8 C
-0.488 -0.156 -0.176
-0.156 -0.560 -0.026
-0.176 -0.026 -1.859
0.000 0.002 0.000

0.001 0.001 0.000
0.000 0.000 0.001

atensor 9 C
-0.675 -0.243 0.152
-0.243 -0.539 0.066
0.152 0.066 0.411
-0.006 -0.003 0.001
0.006 0.003 -0.001
0.001 0.000 0.001

atensor 10 C
1.182 -1.044 -0.286
-1.044 0.966 0.057
-0.286 0.057 -1.265
-0.004 0.010 0.001
0.008 -0.004 -0.001
0.001 -0.001 0.009

atensor 11 C
-0.859 -1.742 0.007
-1.742 -3.282 0.294
0.007 0.294 -1.279
0.091 0.036 0.000
-0.018 -0.032 0.007
0.002 0.000 0.100

atensor 12 C
-0.125 -0.594 0.046
-0.594 1.966 -2.215
0.046 -2.215 1.180
0.091 -0.002 0.006
0.009 -0.005 0.070
0.000 0.049 0.073

atensor 13 C
1.492 1.625 -0.903
1.625 -0.552 -1.003
-0.903 -1.003 0.670
0.053 -0.029 0.003
-0.045 0.011 0.033
0.009 0.034 0.084

atensor 14 C
-0.062 -0.008 0.263
-0.008 2.277 2.217
0.263 2.217 0.812
0.088 -0.014 -0.008
-0.009 -0.013 -0.065
-0.003 -0.041 0.083

atensor 15 C
-0.255 -0.228 0.292
-0.228 0.261 -0.816
0.292 -0.816 0.799
0.013 0.001 -0.007
0.000 0.001 0.007
-0.005 0.011 -0.002

atensor 16 H
-0.506 -0.171 0.190
-0.171 0.995 -1.472
0.190 -1.472 0.883
0.007 0.004 -0.005
0.000 -0.002 0.011
-0.001 0.017 -0.004

atensor 17 H
-0.310 -1.300 1.608
-1.300 -0.124 -1.831
1.608 -1.831 0.680
0.005 0.013 -0.017
0.007 0.001 0.015
-0.019 0.025 -0.008

atensor 18 H
-1.896 -0.241 0.541
-0.241 -1.196 -1.889
0.541 -1.889 3.148
0.016 -0.002 -0.012
-0.004 0.014 0.011
-0.004 0.027 -0.038

atensor 19 C
0.579 0.450 -0.633
0.450 0.125 -0.394
-0.633 -0.394 0.450
0.003 -0.006 0.007
-0.004 0.004 0.001
0.010 0.005 0.005

atensor 20 H
-0.879 0.984 -0.891
0.984 -0.842 -0.910
-0.891 -0.910 -0.992
0.003 -0.008 0.005
-0.006 0.004 0.005
0.009 0.010 0.003

atensor 21 H
-0.371 0.810 -2.417
0.810 -1.830 -1.064
-2.417 -1.064 1.147
0.004 -0.009 0.019
-0.001 0.016 0.000
0.030 0.017 -0.017

atensor 22 H
1.623 1.159 -1.521
1.159 -1.212 -0.566
-1.521 -0.566 -0.834
-0.010 -0.014 0.013
-0.004 0.012 0.002
0.018 0.008 0.010

atensor 23 C
0.874 0.576 0.479
0.576 0.172 0.269
0.479 0.269 0.110
0.000 -0.007 -0.005
-0.005 0.004 0.001
-0.008 -0.003 0.009

atensor 24 C
-0.331 -0.018 0.000
-0.018 0.378 0.880
0.000 0.880 0.757
0.015 -0.001 0.002
-0.002 -0.001 -0.007
0.001 -0.011 -0.003

atensor 25 H
-0.509 0.207 0.150
0.207 1.201 1.447

0.150 1.448 0.692
0.008 0.000 0.002
-0.003 -0.004 -0.011
-0.002 -0.018 -0.003

atensor 26 H
-1.837 0.293 0.738
0.293 -0.913 2.166
0.738 2.166 2.813
0.016 -0.009 -0.001
-0.007 0.011 -0.013
-0.010 -0.029 -0.036

atensor 27 H
-1.025 -0.876 -1.118
-0.876 0.150 2.178
-1.118 2.178 1.120
0.013 0.007 0.012
0.004 -0.002 -0.018
0.014 -0.028 -0.013

atensor 28 H
1.657 0.553 -0.218
0.553 0.557 -0.087
-0.218 -0.087 0.162
-0.004 -0.007 0.002
-0.003 0.002 0.001
0.002 0.001 0.008

atensor 29 H
0.105 0.234 -0.194
0.234 -1.808 -0.014
-0.194 -0.014 -1.300
-0.007 -0.002 0.002
0.002 0.003 0.000
0.002 0.000 0.005

atensor 30 C
1.849 1.882 0.452
1.882 -0.448 0.610
0.452 0.610 0.196
0.053 -0.036 0.008
-0.052 0.008 -0.015
0.003 -0.021 0.088

atensor 31 H
2.191 1.340 0.627
1.340 -1.156 0.240
0.627 0.240 -1.458
-0.016 -0.016 -0.005
-0.005 0.012 0.000
-0.011 -0.004 0.017

atensor 32 H
0.898 1.243 2.392
1.243 -1.693 0.949
2.392 0.949 -0.267
-0.009 -0.015 -0.020
-0.003 0.015 -0.001
-0.031 -0.015 -0.002

atensor 33 H
-0.473 1.235 0.660
1.235 -0.743 0.589
0.660 0.589 -1.511
0.000 -0.011 -0.004
-0.008 0.003 -0.004

-0.007 -0.007 0.007

atensor 34 H
-0.865 3.518 -0.510
3.518 1.095 -0.629
-0.510 -0.629 -3.759
0.009 -0.033 0.006
-0.023 -0.007 0.005
0.005 0.006 0.042

atensor 35 H
0.099 -0.250 -0.115
-0.250 -0.987 0.037
-0.115 0.037 -0.839
-0.005 0.002 0.001
0.002 0.001 0.000
0.001 0.000 0.004

atensor 36 H
0.723 -0.235 -0.073
-0.235 0.444 0.019
-0.073 0.019 0.107
-0.003 0.004 0.001
0.003 -0.001 0.000
0.001 0.000 0.003

atensor 37 H
-0.757 -0.609 -0.003
-0.609 0.416 0.032
-0.003 0.032 -0.946
-0.001 0.008 0.001
0.006 -0.006 0.000
0.001 -0.001 0.007

atensor 38 Cr
30.601 3.477 -0.392
3.477 40.592 -0.868
-0.392 -0.868 28.577
3.930 -0.623 0.148
-0.679 2.801 0.161
0.150 0.154 4.881

atensor 39 Cl
5.893 0.342 1.317
0.342 2.820 -4.294
1.317 -4.294 -3.518
0.459 0.030 0.039
-0.001 0.205 -0.124
0.015 -0.289 0.259

atensor 40 Cl
4.602 1.203 -3.594
1.203 3.664 3.655
-3.594 3.655 -2.774
0.432 0.099 -0.093
0.029 0.233 0.123
-0.065 0.275 0.259

orbtensor 1 N
-478.421 37.800 58.006
37.800 -529.028 12.750
58.006 12.750 -29.102
320.744 -4.183 -3.987
-4.183 334.554 -1.042
-3.987 -1.042 289.493

orbtensor 2 C

-292.975	32.052	27.309
32.052	-332.570	4.835
27.309	4.835	-77.390
258.152	6.195	-4.410
6.195	262.226	-2.070
-4.410	-2.070	226.518

orbtensor 3 C

-229.836	-46.014	26.614
-46.014	-277.394	14.315
26.614	14.315	-41.595
255.842	-0.895	-5.272
-0.895	253.738	-1.231
-5.272	-1.231	215.759

orbtensor 4 C

-317.413	-29.314	35.628
-29.314	-253.117	10.855
35.628	10.855	-56.379
251.601	3.779	-4.169
3.779	262.605	-1.956
-4.169	-1.956	221.137

orbtensor 5 C

-295.581	2.264	33.339
2.264	-275.138	7.979
33.339	7.979	-42.188
272.067	1.917	-5.793
1.917	258.902	-1.326
-5.793	-1.326	228.777

orbtensor 6 C

-292.153	14.945	25.230
14.945	-324.705	6.027
25.230	6.027	-98.220
269.754	0.621	-4.861
0.621	269.659	-1.373
-4.861	-1.373	233.161

orbtensor 7 C

-305.851	18.660	32.016
18.660	-221.023	3.369
32.016	3.369	-59.096
254.058	-5.895	-4.280
-5.895	260.351	-0.659
-4.280	-0.659	220.090

orbtensor 8 C

-260.113	49.604	25.991
49.604	-276.393	1.521
25.991	1.521	-50.084
258.434	3.078	-4.701
3.078	257.517	-1.602
-4.701	-1.602	223.716

orbtensor 9 C

-251.091	-39.939	27.779
-39.939	-293.682	13.686
27.779	13.686	-51.594
258.164	-5.429	-5.255
-5.429	252.581	-0.561
-5.255	-0.561	216.925

orbtensor 10 C

-310.633	-22.422	31.751
-22.422	-245.558	8.861
31.751	8.861	-76.892

268.499	2.770	-5.340
2.770	261.156	-1.511
-5.340	-1.511	228.841

orbtensor 11 C

-230.852	34.773	1.022
34.773	-113.263	-8.102
1.022	-8.102	-213.293
258.457	-2.889	-0.375
-2.889	229.154	1.255
-0.375	1.255	254.801

orbtensor 12 C

-209.785	26.600	0.540
26.600	-99.860	28.452
0.540	28.452	-238.823
264.787	-4.145	-5.487
-4.145	237.688	-1.551
-5.487	-1.551	256.094

orbtensor 13 C

-247.839	1.930	11.754
1.930	-86.222	14.085
11.754	14.085	-236.640
261.878	-1.720	5.225
-1.720	236.035	-1.009
5.225	-1.009	260.725

orbtensor 14 C

-212.167	16.984	-8.496
16.984	-104.683	-43.376
-8.496	-43.376	-231.383
266.986	-3.170	2.833
-3.170	238.051	3.657
2.833	3.657	253.536

orbtensor 15 C

-43.168	2.306	2.594
2.306	-36.536	4.185
2.594	4.185	-42.804
215.199	-1.373	4.957
-1.373	212.112	-4.262
4.957	-4.262	226.871

orbtensor 16 H

3.443	-0.603	-0.438
-0.603	3.075	1.373
-0.438	1.373	1.707
23.626	1.004	-0.318
1.004	28.541	-6.508
-0.318	-6.508	29.322

orbtensor 17 H

3.260	0.569	-2.985
0.569	3.308	2.641
-2.985	2.641	2.216
31.045	-0.746	0.857
-0.746	21.019	-2.089
0.857	-2.089	29.597

orbtensor 18 H

5.756	0.177	-0.914
0.177	4.833	2.388
-0.914	2.388	-2.608
21.653	-2.585	-0.196
-2.585	25.798	1.833
-0.196	1.833	31.053

orbtensor 19 C
-41.914 -2.139 -1.803
-2.139 -32.689 2.609
-1.803 2.609 -44.249
221.944 1.392 -9.219
1.392 211.213 -0.282
-9.219 -0.282 219.217

orbtensor 20 H
3.034 -0.657 1.313
-0.657 3.411 0.669
1.313 0.669 2.916
26.520 3.261 -4.213
3.261 28.117 -4.741
-4.213 -4.741 26.546

orbtensor 21 H
2.773 -1.483 3.955
-1.483 5.222 0.951
3.955 0.951 -0.401
25.867 2.576 -3.261
2.576 24.290 3.579
-3.261 3.579 29.100

orbtensor 22 H
-1.274 -1.299 2.413
-1.299 3.008 0.909
2.413 0.909 3.912
34.228 -1.920 -1.153
-1.920 22.679 -0.769
-1.153 -0.769 26.220

orbtensor 23 C
-41.128 -2.685 1.177
-2.685 -32.992 -2.687
1.177 -2.687 -44.669
226.284 2.041 7.229
2.041 211.253 0.225
7.229 0.225 214.833

orbtensor 24 C
-44.449 0.954 -2.171
0.954 -37.229 -4.901
-2.171 -4.901 -40.902
213.521 -0.328 -1.458
-0.328 212.784 5.527
-1.458 5.527 227.879

orbtensor 25 H
3.542 -0.938 0.040
-0.938 2.835 -1.227
0.040 -1.227 1.766
24.102 2.690 1.445
2.690 29.410 6.011
1.445 6.011 27.976

orbtensor 26 H
5.661 -0.506 -1.204
-0.506 4.407 -2.862
-1.204 -2.862 -2.161
22.422 -2.821 2.697
-2.821 25.612 -0.770
2.697 -0.770 30.475

orbtensor 27 H
4.639 0.038 2.367

0.038	2.867	-2.820
2.367	-2.820	1.187
30.531	-0.173	-1.113
-0.173	21.354	2.793
-1.113	2.793	29.774

orbtensor 28 H

-4.720	-6.622	0.621
-6.622	-15.396	1.338
0.621	1.338	-1.844
31.124	5.238	-1.379
5.238	40.783	-1.338
-1.379	-1.338	22.138

orbtensor 29 H

-18.999	-3.568	2.204
-3.568	-2.751	0.443
2.204	0.443	-3.249
41.577	2.890	-2.696
2.890	30.270	-0.678
-2.696	-0.678	21.972

orbtensor 30 C

-252.860	-3.702	-7.127
-3.702	-88.938	-23.940
-7.127	-23.940	-229.015
259.249	-1.527	-4.754
-1.527	236.318	3.203
-4.754	3.203	263.062

orbtensor 31 H

-2.089	-1.582	-0.702
-1.582	2.861	-0.407
-0.702	-0.407	4.827
34.306	-1.619	-0.874
-1.619	22.831	1.449
-0.874	1.449	25.991

orbtensor 32 H

0.622	-2.016	-4.091
-2.016	5.089	-0.803
-4.091	-0.803	1.847
27.656	1.854	3.554
1.854	23.783	-3.849
3.554	-3.849	27.816

orbtensor 33 H

2.383	-0.876	-1.098
-0.876	3.276	-0.450
-1.098	-0.450	3.632
28.520	4.600	3.336
4.600	28.685	3.502
3.336	3.502	23.974

orbtensor 34 H

-6.658	5.700	0.671
5.700	-13.888	-0.259
0.671	-0.259	0.042
33.766	-3.339	-1.802
-3.339	35.943	-0.156
-1.802	-0.156	19.225

orbtensor 35 H

-18.943	1.012	2.024
1.012	-2.882	-0.129
2.024	-0.129	-3.335
42.730	-0.875	-2.654

-0.875 30.412 -0.178
 -2.654 -0.178 22.407

orbtensor 36 H
 -7.272 7.824 0.308
 7.824 -13.384 -0.647
 0.308 -0.647 -2.836
 33.497 -6.652 -1.196
 -6.652 38.506 0.305
 -1.196 0.305 22.643

orbtensor 37 H
 -4.379 -6.099 0.625
 -6.099 -16.042 1.306
 0.625 1.306 -1.231
 31.016 2.404 -1.403
 2.404 39.908 -0.975
 -1.403 -0.975 21.071

orbtensor 38 Cr
 -6004.070 853.540 -165.268
 853.540 -4214.931 -208.875
 -165.268 -208.875 -7020.271
 1805.955 2.281 -0.386
 2.281 1813.332 -0.632
 -0.386 -0.632 1803.663

orbtensor 39 Cl
 -11.457 -11.543 26.108
 -11.543 -151.844 0.994
 26.108 0.994 -121.979
 1141.748 -0.588 -2.081
 -0.588 1145.692 4.904
 -2.081 4.904 1146.300

orbtensor 40 Cl
 -31.253 -13.605 -49.201
 -13.605 -151.432 4.906
 -49.201 4.906 -102.257
 1143.105 -1.638 3.092
 -1.638 1145.041 -4.571
 3.092 -4.571 1145.592

gtensor (ppt)
 -0.169 0.006 0.000
 0.006 -0.155 -0.001
 0.000 -0.001 -0.170
 -16.478 5.017 -1.296
 5.017 -12.327 -1.095
 -1.296 -1.095 -24.914

zfstensor (cm-1)
 -0.792143 0.457143 -0.030842
 0.457143 0.797254 -0.115208
 -0.030842 -0.115208 -0.919196

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.2587	-30.58667	5919.44085	-2.13856	5917.30229	5886.71563
2	C	3.5437	14.65367	-1850.10418	-0.51330	-1850.61748	-1835.96381
3	C	-1.2607	58.83800	658.17835	-0.37793	657.80042	716.63842
4	C	1.5637	36.14467	-816.37087	-0.31453	-816.68539	-780.54073
5	C	-1.4897	48.94633	777.73639	-0.35897	777.37742	826.32375
6	C	0.6977	19.16533	-364.24307	-1.37029	-365.61335	-346.44802
7	C	0.8593	49.50967	-448.64722	-0.18429	-448.83151	-399.32184

8	C	-0.9683	51.02567	505.55476	-0.07262	505.48214	556.50781
9	C	-0.2683	43.76767	140.09349	0.09715	140.19063	183.95830
10	C	0.2947	41.80433	-153.84179	-0.21804	-154.05983	-112.25549
11	C	-1.7537	61.66800	915.56750	-1.67054	913.89696	975.56496
12	C	1.0600	70.03367	-553.41278	1.30598	-552.10680	-482.07314
13	C	0.5860	62.64567	-305.94329	-1.33433	-307.27762	-244.63195
14	C	1.0617	70.11333	-554.28293	1.34338	-552.93955	-482.82622
15	C	0.2723	177.22467	-142.18184	0.37905	-141.80279	35.42188
16	H	0.4577	29.90467	-60.09484	0.25286	-59.84199	-29.93732
17	H	0.0813	30.14833	-10.67964	0.09772	-10.58192	19.56641
18	H	0.0160	28.82833	-2.10091	0.14199	-1.95892	26.86941
19	C	0.3887	177.84067	-202.91802	-0.34932	-203.26734	-25.42667
20	H	-0.9010	30.18133	118.30762	-0.01065	118.29697	148.47831
21	H	-0.3503	28.95033	46.00122	-0.30823	45.69299	74.64332
22	H	-0.1370	29.59100	17.98906	-0.48185	17.50721	47.09821
23	C	0.3897	177.86033	-203.44011	-0.33875	-203.77886	-25.91853
24	C	0.2717	177.20133	-141.83378	0.39052	-141.44326	35.75807
25	H	0.4617	29.87700	-60.62007	0.25840	-60.36167	-30.48467
26	H	0.0180	28.80533	-2.36353	0.15019	-2.21333	26.59200
27	H	0.0810	30.11733	-10.63587	0.10154	-10.53433	19.58300
28	H	0.7940	24.02833	-104.25777	-0.17163	-104.42939	-80.40106
29	H	-1.0007	22.94000	131.39455	-0.30165	131.09290	154.03290
30	C	0.5820	62.60533	-303.85494	-1.31825	-305.17319	-242.56786
31	H	-0.1367	29.57567	17.94529	-0.47750	17.46779	47.04346
32	H	-0.3527	28.93767	46.30761	-0.29818	46.00943	74.94709
33	H	-0.9057	30.15667	118.92038	-0.00576	118.91462	149.07129
34	H	-1.1617	22.81000	152.53498	0.33189	152.86687	175.67687
35	H	-0.5757	23.46300	75.58907	-0.17592	75.41315	98.87615
36	H	0.4243	23.71800	-55.71794	-0.04841	-55.76636	-32.04836
37	H	-0.4290	23.44767	56.33071	0.17608	56.50678	79.95445
38	Cr	37.1273	-3938.77400	86075.05421	-25.03136	86050.02285	82111.24885
39	Cl	2.0393	1049.48667	-2729.85256	-4.11669	-2733.96925	-1684.48258
40	Cl	2.0387	1049.59867	-2728.96016	-4.01922	-2732.97938	-1683.38072

=====
CrL1-STO-BP-No-ZFS

Temperature: 295

Spin: 1.5

atensor 1 N

-1.397 0.228 -0.236
0.228 -2.244 -0.061
-0.236 -0.061 -3.118
-0.011 0.030 0.003
-0.003 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.752 0.953 0.423
0.953 1.883 0.029
0.423 0.029 6.211
-0.048 0.013 0.006
0.013 0.006 -0.002
0.006 -0.002 0.003

atensor 3 C

0.210 0.161 -0.276
0.161 -0.437 -0.071
-0.276 -0.071 -1.834
0.001 -0.009 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C

0.125 0.072 0.533
0.072 -0.462 0.155

0.533 0.155 4.169
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.632 -0.093 -0.134
-0.093 -1.080 -0.009
-0.134 -0.009 -1.673
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.338 -0.515 -0.057
-0.515 -0.701 0.118
-0.057 0.118 0.770
0.007 0.000 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.114 -0.110 0.090
-0.110 -0.144 0.046
0.090 0.046 0.765
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.147 -0.154 -0.071
-0.154 -0.219 0.002
-0.071 0.002 -0.727
0.000 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.114 -0.245 0.131
-0.245 -0.968 0.060
0.131 0.060 -0.190
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.235 -0.950 -0.180
-0.950 0.978 0.076
-0.180 0.076 -0.382
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.004

atensor 11 C
0.213 -1.559 0.008
-1.559 -1.769 0.257
0.008 0.258 -0.149
0.059 0.019 0.002
-0.008 -0.015 0.004
0.003 0.001 0.082

atensor 12 C
0.227 -0.329 -0.008
-0.329 2.532 -2.301
-0.008 -2.301 1.365
0.060 0.000 0.000
-0.010 0.001 0.030

-0.008 0.027 0.043

atensor 13 C
1.911 1.560 -0.818
1.560 0.349 -1.040
-0.818 -1.041 1.168
0.039 -0.013 0.003
-0.029 0.011 0.021
0.005 0.018 0.065

atensor 14 C
0.300 0.267 0.250
0.267 2.845 2.207
0.250 2.207 0.980
0.061 -0.007 -0.004
-0.016 -0.003 -0.024
0.005 -0.023 0.046

atensor 15 C
-0.020 -0.220 0.287
-0.220 0.438 -0.792
0.287 -0.792 1.044
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.130 -0.140 0.191
-0.140 1.601 -1.417
0.191 -1.417 1.469
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.149 -1.225 1.523
-1.225 -0.004 -1.757
1.523 -1.757 0.761
0.003 0.004 -0.006
0.001 0.001 0.007
-0.007 0.012 -0.003

atensor 18 H
-1.740 -0.233 0.505
-0.233 -0.951 -1.805
0.505 -1.805 3.060
0.005 -0.003 -0.007
-0.003 0.008 0.004
0.000 0.013 -0.017

atensor 19 C
0.542 0.421 -0.618
0.421 0.072 -0.374
-0.618 -0.374 0.443
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.477 0.938 -0.868
0.938 -0.434 -0.862
-0.868 -0.862 -0.597
0.003 -0.003 0.000
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H

-0.224 0.814 -2.299
0.814 -1.531 -1.016
-2.299 -1.016 1.182
0.003 -0.003 0.006
0.001 0.009 -0.001
0.012 0.009 -0.006

atensor 22 H
1.624 1.099 -1.450
1.099 -1.082 -0.541
-1.450 -0.541 -0.747
0.000 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.831 0.542 0.476
0.542 0.116 0.260
0.476 0.260 0.109
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.090 -0.015 0.006
-0.015 0.554 0.861
0.006 0.861 1.004
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.123 0.222 0.137
0.222 1.799 1.386
0.137 1.386 1.290
0.002 0.001 0.003
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.680 0.277 0.712
0.277 -0.684 2.061
0.712 2.061 2.734
0.005 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.013 -0.016

atensor 27 H
-0.826 -0.818 -1.066
-0.818 0.261 2.083
-1.066 2.083 1.178
0.006 0.001 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.487 0.624 -0.222
0.624 0.535 -0.102
-0.222 -0.102 -0.021
0.000 -0.005 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
-0.073 0.282 -0.224
0.282 -2.559 -0.008
-0.224 -0.008 -1.694

-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.234 1.821 0.401
1.821 0.461 0.637
0.401 0.637 0.728
0.039 -0.017 0.005
-0.033 0.009 -0.009
0.004 -0.011 0.067

atensor 31 H
2.163 1.272 0.591
1.272 -1.028 0.230
0.591 0.230 -1.341
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.007

atensor 32 H
0.981 1.224 2.263
1.224 -1.401 0.887
2.263 0.887 -0.158
-0.002 -0.006 -0.006
0.000 0.009 0.000
-0.013 -0.008 -0.001

atensor 33 H
-0.081 1.176 0.643
1.176 -0.340 0.555
0.643 0.555 -1.100
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.378 2.944 -0.452
2.944 0.407 -0.539
-0.452 -0.539 -3.994
0.010 -0.001 0.002
-0.009 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.192 -0.289 -0.111
-0.289 -0.720 0.037
-0.111 0.037 -0.723
-0.001 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.337 -0.372 -0.060
-0.372 0.152 0.035
-0.060 0.035 -0.219
-0.001 0.002 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.558 -0.586 -0.010
-0.586 0.537 0.030
-0.010 0.030 -0.794
-0.002 0.001 0.000
0.002 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.863 2.936 -0.258
2.936 27.658 -0.725
-0.258 -0.725 17.715
2.429 -0.364 0.113
-0.384 2.040 0.090
0.113 0.087 3.182

atensor 39 Cl
6.351 0.146 1.824
0.146 2.731 -4.905
1.824 -4.905 -6.066
0.474 0.039 0.038
0.036 0.256 -0.190
0.006 -0.267 0.347

atensor 40 Cl
4.614 1.091 -4.778
1.091 3.350 4.144
-4.778 4.144 -4.950
0.453 0.102 -0.075
0.082 0.286 0.180
-0.042 0.254 0.337

orbtensor 1 N
-476.767 51.958 48.516
51.958 -551.690 9.313
48.516 9.313 -96.157
338.521 -2.790 -2.014
-2.790 352.359 -0.683
-2.014 -0.683 322.569

orbtensor 2 C
-269.772 25.851 25.162
25.851 -298.646 4.626
25.162 4.626 -72.625
253.092 6.157 -5.665
6.157 252.127 -2.226
-5.665 -2.226 211.962

orbtensor 3 C
-222.771 -47.342 23.622
-47.342 -286.652 14.261
23.622 14.261 -57.225
252.337 3.889 -3.913
3.889 263.144 -1.894
-3.913 -1.894 223.832

orbtensor 4 C
-301.509 -22.132 32.894
-22.132 -231.418 9.044
32.894 9.044 -58.839
257.133 3.287 -5.268
3.287 253.321 -1.676
-5.268 -1.676 218.207

orbtensor 5 C
-287.597 2.684 30.137
2.684 -276.312 7.364
30.137 7.364 -59.009
269.078 0.621 -4.475
0.621 266.926 -1.201
-4.475 -1.201 235.409

orbtensor 6 C
-273.672 19.767 22.021

19.767	-298.093	4.353
22.021	4.353	-101.825
263.297	-4.674	-5.740
-4.674	261.723	-0.917
-5.740	-0.917	218.637

orbtensor 7 C

-295.829	12.610	30.563
12.610	-210.969	3.731
30.563	3.731	-61.195
257.851	-4.101	-5.085
-4.101	252.330	-0.679
-5.085	-0.679	218.275

orbtensor 8 C

-247.413	53.705	24.004
53.705	-272.020	0.832
24.004	0.832	-51.239
253.687	-5.371	-4.182
-5.371	256.250	-0.566
-4.182	-0.566	220.595

orbtensor 9 C

-236.953	-36.098	24.846
-36.098	-289.836	12.853
24.846	12.853	-58.877
253.125	-3.421	-4.280
-3.421	257.730	-0.897
-4.280	-0.897	219.825

orbtensor 10 C

-302.885	-14.652	28.573
-14.652	-250.073	7.595
28.573	7.595	-90.683
270.314	-0.813	-4.470
-0.813	265.280	-0.927
-4.470	-0.927	236.273

orbtensor 11 C

-220.827	33.177	0.122
33.177	-134.300	-6.951
0.122	-6.951	-210.845
250.310	-7.752	-1.266
-7.752	241.165	0.911
-1.266	0.911	238.629

orbtensor 12 C

-199.453	20.524	0.690
20.524	-106.842	24.199
0.690	24.199	-237.466
244.041	-2.650	-4.723
-2.650	236.024	-6.038
-4.723	-6.038	246.231

orbtensor 13 C

-228.891	-1.967	14.484
-1.967	-94.590	13.419
14.484	13.419	-220.823
247.773	3.495	-2.403
3.495	233.252	-4.285
-2.403	-4.285	245.876

orbtensor 14 C

-202.472	12.149	-10.569
12.149	-111.077	-37.099
-10.569	-37.099	-230.176
246.527	-0.617	4.642

-0.617 236.930 7.016
4.642 7.016 242.838

orbtensor 15 C
-56.470 0.997 6.681
0.997 -48.559 2.873
6.681 2.873 -50.088
219.885 -0.322 2.564
-0.322 218.624 -4.258
2.564 -4.258 228.708

orbtensor 16 H
2.962 -0.721 0.101
-0.721 1.912 1.407
0.101 1.407 1.266
23.784 0.874 -0.628
0.874 29.299 -6.778
-0.628 -6.778 29.501

orbtensor 17 H
3.054 0.384 -1.960
0.384 3.379 2.362
-1.960 2.362 2.605
30.497 -0.478 0.421
-0.478 20.916 -2.417
0.421 -2.417 29.051

orbtensor 18 H
5.022 0.265 -0.055
0.265 3.316 2.180
-0.055 2.180 -1.453
21.577 -2.496 -0.447
-2.496 26.719 1.350
-0.447 1.350 30.585

orbtensor 19 C
-54.157 -0.468 -5.666
-0.468 -46.188 2.624
-5.666 2.624 -55.366
226.851 0.725 -6.853
0.725 218.951 -1.278
-6.853 -1.278 223.738

orbtensor 20 H
2.078 -0.616 1.178
-0.616 2.017 0.835
1.178 0.835 2.205
26.999 3.474 -4.146
3.474 28.744 -5.104
-4.146 -5.104 26.847

orbtensor 21 H
2.335 -1.557 2.987
-1.557 3.830 0.890
2.987 0.890 0.222
25.919 2.911 -3.047
2.911 25.013 3.340
-3.047 3.340 28.585

orbtensor 22 H
-1.384 -0.860 1.455
-0.860 2.919 1.122
1.455 1.122 3.523
33.936 -2.111 -0.718
-2.111 22.554 -1.227
-0.718 -1.227 26.121

orbtensor 23 C
-51.425 -0.852 4.722
-0.852 -46.581 -3.159
4.722 -3.159 -57.708
230.007 1.472 5.098
1.472 219.126 1.194
5.098 1.194 220.408

orbtensor 24 C
-59.344 -0.148 -4.210
-0.148 -48.965 -2.956
-4.210 -2.956 -46.792
219.178 0.770 -0.147
0.770 219.255 4.888
-0.147 4.888 228.779

orbtensor 25 H
2.820 -1.078 -0.422
-1.078 1.729 -1.201
-0.422 -1.201 1.589
24.415 2.648 1.722
2.648 30.204 6.255
1.722 6.255 27.964

orbtensor 26 H
4.631 -0.390 -1.507
-0.390 2.994 -2.463
-1.507 -2.463 -0.741
22.440 -2.614 2.801
-2.614 26.589 -0.430
2.801 -0.430 29.854

orbtensor 27 H
3.998 -0.114 1.628
-0.114 3.047 -2.462
1.628 -2.462 1.997
30.190 0.192 -0.759
0.192 21.289 2.998
-0.759 2.998 28.982

orbtensor 28 H
-5.777 -6.386 0.619
-6.386 -16.718 1.316
0.619 1.316 -2.851
32.096 5.149 -1.294
5.149 41.605 -1.299
-1.294 -1.299 23.732

orbtensor 29 H
-18.504 -2.662 2.281
-2.662 -3.478 0.409
2.281 0.409 -1.965
41.673 2.199 -2.712
2.199 30.611 -0.607
-2.712 -0.607 21.760

orbtensor 30 C
-235.404 -7.251 -10.039
-7.251 -96.936 -20.510
-10.039 -20.510 -211.983
248.756 4.705 1.279
4.705 233.828 4.010
1.279 4.010 244.323

orbtensor 31 H
-1.762 -1.159 0.030
-1.159 2.788 -0.790

0.030	-0.790	4.033
33.813	-1.714	-1.205
-1.714	22.772	1.950
-1.205	1.950	26.028

orbtensor 32 H

0.752	-1.966	-2.990
-1.966	3.723	-0.620
-2.990	-0.620	1.907
27.559	2.209	3.202
2.209	24.528	-3.781
3.202	-3.781	27.428

orbtensor 33 H

1.519	-0.878	-0.931
-0.878	1.917	-0.601
-0.931	-0.601	2.862
28.951	4.889	3.212
4.889	29.357	3.775
3.212	3.775	24.283

orbtensor 34 H

-8.215	3.713	0.856
3.713	-14.390	-0.003
0.856	-0.003	-0.751
34.829	-1.316	-1.911
-1.316	36.463	-0.411
-1.911	-0.411	20.016

orbtensor 35 H

-18.329	0.609	2.094
0.609	-3.406	-0.031
2.094	-0.031	-2.308
42.213	-0.596	-2.651
-0.596	30.454	-0.230
-2.651	-0.230	21.988

orbtensor 36 H

-8.095	7.662	0.355
7.662	-13.776	-0.629
0.355	-0.629	-3.327
34.069	-6.703	-1.154
-6.703	38.535	0.341
-1.154	0.341	23.515

orbtensor 37 H

-5.360	-5.153	0.654
-5.153	-16.460	1.184
0.654	1.184	-1.827
31.636	1.659	-1.305
1.659	40.316	-0.852
-1.305	-0.852	22.234

orbtensor 38 Cr

-4995.561	438.282	-76.226
438.282	-3640.003	-119.878
-76.226	-119.878	-5452.191
1814.620	1.011	-0.424
1.011	1814.563	-0.233
-0.424	-0.233	1811.689

orbtensor 39 Cl

-322.415	-20.258	15.031
-20.258	-460.519	164.382
15.031	164.382	-394.034
1141.122	-0.744	-2.553
-0.744	1145.107	5.235

-2.553 5.235 1146.575

orbtensor 40 C1

-333.399 -62.189 -25.241
-62.189 -482.016 -147.288
-25.241 -147.288 -361.469
1142.777 -1.828 3.741
-1.828 1144.418 -4.803
3.741 -4.803 1145.611

gtensor (ppt)

-0.152 0.005 -0.001
0.005 -0.153 -0.001
-0.001 -0.001 -0.154
-3.907 3.399 -0.902
3.399 -2.988 -0.682
-0.902 -0.682 -9.807

averaging

2H Average:34
3H Average:28
4H Average:29
5H Average:35
6H Average:36
7H Average:37
8,11H Average:25,26,27,31,32,33
9,10H Average:16,17,18,20,21,22

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.2393	-37.05500	4093.17705	-2.20585	4090.97119	4053.91619
2	C	3.6023	25.37933	-1892.46674	0.98425	-1891.48249	-1866.10316
3	C	-0.6890	57.55500	361.96250	-0.75798	361.20452	418.75952
4	C	1.2713	45.63167	-667.88823	1.69891	-666.18932	-620.55765
5	C	-1.1263	49.49833	591.71325	-0.25195	591.46130	640.95963
6	C	0.4670	23.35567	-245.33598	0.57092	-244.76505	-221.40939
7	C	0.2437	53.48767	-128.00899	0.38655	-127.62244	-74.13478
8	C	-0.3647	53.28667	191.57570	-0.12011	191.45559	244.74226
9	C	-0.7590	48.33800	398.73663	0.48788	399.22451	447.56251
10	C	0.6087	42.74200	-319.75981	0.00763	-319.75218	-277.01018
11	C	-0.5263	54.71067	276.50643	1.29945	277.80588	332.51655
12	C	1.4093	60.84500	-740.38580	-0.16589	-740.55169	-679.70669
13	C	1.1810	60.86567	-620.43210	-1.07719	-621.50928	-560.64361
14	C	1.4097	60.85667	-740.56092	-0.16521	-740.72613	-679.86946
15	C	0.4917	170.70000	-258.29448	0.37325	-257.92123	-87.22123
16	H	1.0670	29.57467	-140.97866	0.02730	-140.95136	-111.37669
17	H	0.2030	29.83400	-26.82162	0.26777	-26.55385	3.28015
18	H	0.1217	28.58867	-16.07535	0.40317	-15.67218	12.91649
19	C	0.3563	171.27633	-187.19783	-0.32090	-187.51872	-16.24239
20	H	-0.5007	29.63000	66.15119	-0.21458	65.93661	95.56661
21	H	-0.1890	28.63467	24.97185	-0.03911	24.93274	53.56741
22	H	-0.0647	29.22300	8.54416	-0.30590	8.23827	37.46127
23	C	0.3560	171.27567	-187.02271	-0.32018	-187.34290	-16.06723
24	C	0.4937	170.70367	-259.34517	0.37333	-258.97184	-88.26818
25	H	1.0710	29.57367	-141.50717	0.02753	-141.47964	-111.90597
26	H	0.1220	28.58900	-16.11940	0.40342	-15.71598	12.87302
27	H	0.2043	29.83433	-26.99779	0.26793	-26.72986	3.10447
28	H	0.6680	24.02900	-88.26030	-0.19168	-88.45199	-64.42299
29	H	-1.4423	23.36567	190.57003	-0.06139	190.50864	213.87431
30	C	1.1793	60.86133	-619.55652	-1.07489	-620.63141	-559.77008
31	H	-0.0653	29.22400	8.63225	-0.30580	8.32645	37.55045
32	H	-0.1907	28.63233	25.19206	-0.03853	25.15353	53.78586
33	H	-0.5050	29.62967	66.72373	-0.21427	66.50946	96.13913
34	H	-1.6450	22.65067	217.34761	-0.81980	216.52781	239.17847
35	H	-0.4167	23.53733	55.05259	0.00646	55.05905	78.59638

36	H	0.0897	23.64033	-11.84732	0.01301	-11.83431	11.80602
37	H	-0.2727	23.51300	36.02641	0.00434	36.03075	59.54375
38	Cr	23.9623	-2882.29433	55900.24240	16.33056	55916.57296	53034.27863
39	Cl	1.3643	751.94533	-1837.69106	-10.84416	-1848.53521	-1096.58988
40	Cl	1.3633	751.97400	-1836.34410	-10.83671	-1847.18082	-1095.20682

=====
CrL1-STO-BP-Neese

Temperature: 295

Spin: 1.5

atensor 1 N

-1.397 0.228 -0.236
0.228 -2.244 -0.061
-0.236 -0.061 -3.118
-0.011 0.030 0.003
-0.003 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.752 0.953 0.423
0.953 1.883 0.029
0.423 0.029 6.211
-0.048 0.013 0.006
0.013 0.006 -0.002
0.006 -0.002 0.003

atensor 3 C

0.210 0.161 -0.276
0.161 -0.437 -0.071
-0.276 -0.071 -1.834
0.001 -0.009 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C

0.125 0.072 0.533
0.072 -0.462 0.155
0.533 0.155 4.169
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C

-0.632 -0.093 -0.134
-0.093 -1.080 -0.009
-0.134 -0.009 -1.673
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C

1.338 -0.515 -0.057
-0.515 -0.701 0.118
-0.057 0.118 0.770
0.007 0.000 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C

0.114 -0.110 0.090
-0.110 -0.144 0.046
0.090 0.046 0.765
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.147 -0.154 -0.071
-0.154 -0.219 0.002
-0.071 0.002 -0.727
0.000 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.114 -0.245 0.131
-0.245 -0.968 0.060
0.131 0.060 -0.190
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.235 -0.950 -0.180
-0.950 0.978 0.076
-0.180 0.076 -0.382
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.004

atensor 11 C
0.213 -1.559 0.008
-1.559 -1.769 0.257
0.008 0.258 -0.149
0.059 0.019 0.002
-0.008 -0.015 0.004
0.003 0.001 0.082

atensor 12 C
0.227 -0.329 -0.008
-0.329 2.532 -2.301
-0.008 -2.301 1.365
0.060 0.000 0.000
-0.010 0.001 0.030
-0.008 0.027 0.043

atensor 13 C
1.911 1.560 -0.818
1.560 0.349 -1.040
-0.818 -1.041 1.168
0.039 -0.013 0.003
-0.029 0.011 0.021
0.005 0.018 0.065

atensor 14 C
0.300 0.267 0.250
0.267 2.845 2.207
0.250 2.207 0.980
0.061 -0.007 -0.004
-0.016 -0.003 -0.024
0.005 -0.023 0.046

atensor 15 C
-0.020 -0.220 0.287
-0.220 0.438 -0.792
0.287 -0.792 1.044
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.130 -0.140 0.191

-0.140 1.601 -1.417
0.191 -1.417 1.469
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.149 -1.225 1.523
-1.225 -0.004 -1.757
1.523 -1.757 0.761
0.003 0.004 -0.006
0.001 0.001 0.007
-0.007 0.012 -0.003

atensor 18 H
-1.740 -0.233 0.505
-0.233 -0.951 -1.805
0.505 -1.805 3.060
0.005 -0.003 -0.007
-0.003 0.008 0.004
0.000 0.013 -0.017

atensor 19 C
0.542 0.421 -0.618
0.421 0.072 -0.374
-0.618 -0.374 0.443
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.477 0.938 -0.868
0.938 -0.434 -0.862
-0.868 -0.862 -0.597
0.003 -0.003 0.000
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.224 0.814 -2.299
0.814 -1.531 -1.016
-2.299 -1.016 1.182
0.003 -0.003 0.006
0.001 0.009 -0.001
0.012 0.009 -0.006

atensor 22 H
1.624 1.099 -1.450
1.099 -1.082 -0.541
-1.450 -0.541 -0.747
0.000 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.831 0.542 0.476
0.542 0.116 0.260
0.476 0.260 0.109
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.090 -0.015 0.006
-0.015 0.554 0.861
0.006 0.861 1.004
0.012 -0.002 0.001

-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.123 0.222 0.137
0.222 1.799 1.386
0.137 1.386 1.290
0.002 0.001 0.003
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.680 0.277 0.712
0.277 -0.684 2.061
0.712 2.061 2.734
0.005 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.013 -0.016

atensor 27 H
-0.826 -0.818 -1.066
-0.818 0.261 2.083
-1.066 2.083 1.178
0.006 0.001 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.487 0.624 -0.222
0.624 0.535 -0.102
-0.222 -0.102 -0.021
0.000 -0.005 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
-0.073 0.282 -0.224
0.282 -2.559 -0.008
-0.224 -0.008 -1.694
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.234 1.821 0.401
1.821 0.461 0.637
0.401 0.637 0.728
0.039 -0.017 0.005
-0.033 0.009 -0.009
0.004 -0.011 0.067

atensor 31 H
2.163 1.272 0.591
1.272 -1.028 0.230
0.591 0.230 -1.341
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.007

atensor 32 H
0.981 1.224 2.263
1.224 -1.401 0.887
2.263 0.887 -0.158
-0.002 -0.006 -0.006
0.000 0.009 0.000
-0.013 -0.008 -0.001

atensor 33 H
-0.081 1.176 0.643
1.176 -0.340 0.555
0.643 0.555 -1.100
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.378 2.944 -0.452
2.944 0.407 -0.539
-0.452 -0.539 -3.994
0.010 -0.001 0.002
-0.009 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.192 -0.289 -0.111
-0.289 -0.720 0.037
-0.111 0.037 -0.723
-0.001 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.337 -0.372 -0.060
-0.372 0.152 0.035
-0.060 0.035 -0.219
-0.001 0.002 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.558 -0.586 -0.010
-0.586 0.537 0.030
-0.010 0.030 -0.794
-0.002 0.001 0.000
0.002 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.863 2.936 -0.258
2.936 27.658 -0.725
-0.258 -0.725 17.715
2.429 -0.364 0.113
-0.384 2.040 0.090
0.113 0.087 3.182

atensor 39 Cl
6.351 0.146 1.824
0.146 2.731 -4.905
1.824 -4.905 -6.066
0.474 0.039 0.038
0.036 0.256 -0.190
0.006 -0.267 0.347

atensor 40 Cl
4.614 1.091 -4.778
1.091 3.350 4.144
-4.778 4.144 -4.950
0.453 0.102 -0.075
0.082 0.286 0.180
-0.042 0.254 0.337

orbtensor 1 N
-476.767 51.958 48.516
51.958 -551.690 9.313

48.516	9.313	-96.157
338.521	-2.790	-2.014
-2.790	352.359	-0.683
-2.014	-0.683	322.569

orbtensor 2 C

-269.772	25.851	25.162
25.851	-298.646	4.626
25.162	4.626	-72.625
253.092	6.157	-5.665
6.157	252.127	-2.226
-5.665	-2.226	211.962

orbtensor 3 C

-222.771	-47.342	23.622
-47.342	-286.652	14.261
23.622	14.261	-57.225
252.337	3.889	-3.913
3.889	263.144	-1.894
-3.913	-1.894	223.832

orbtensor 4 C

-301.509	-22.132	32.894
-22.132	-231.418	9.044
32.894	9.044	-58.839
257.133	3.287	-5.268
3.287	253.321	-1.676
-5.268	-1.676	218.207

orbtensor 5 C

-287.597	2.684	30.137
2.684	-276.312	7.364
30.137	7.364	-59.009
269.078	0.621	-4.475
0.621	266.926	-1.201
-4.475	-1.201	235.409

orbtensor 6 C

-273.672	19.767	22.021
19.767	-298.093	4.353
22.021	4.353	-101.825
263.297	-4.674	-5.740
-4.674	261.723	-0.917
-5.740	-0.917	218.637

orbtensor 7 C

-295.829	12.610	30.563
12.610	-210.969	3.731
30.563	3.731	-61.195
257.851	-4.101	-5.085
-4.101	252.330	-0.679
-5.085	-0.679	218.275

orbtensor 8 C

-247.413	53.705	24.004
53.705	-272.020	0.832
24.004	0.832	-51.239
253.687	-5.371	-4.182
-5.371	256.250	-0.566
-4.182	-0.566	220.595

orbtensor 9 C

-236.953	-36.098	24.846
-36.098	-289.836	12.853
24.846	12.853	-58.877
253.125	-3.421	-4.280
-3.421	257.730	-0.897

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-4.280   -0.897   219.825

orbtensor 10 C
-302.885  -14.652   28.573
-14.652  -250.073   7.595
28.573    7.595  -90.683
270.314   -0.813  -4.470
-0.813   265.280  -0.927
-4.470   -0.927  236.273

orbtensor 11 C
-220.827   33.177    0.122
33.177  -134.300   -6.951
0.122   -6.951  -210.845
250.310  -7.752   -1.266
-7.752  241.165    0.911
-1.266   0.911   238.629

orbtensor 12 C
-199.453   20.524    0.690
20.524  -106.842   24.199
0.690   24.199  -237.466
244.041   -2.650   -4.723
-2.650  236.024   -6.038
-4.723   -6.038   246.231

orbtensor 13 C
-228.891   -1.967   14.484
-1.967  -94.590   13.419
14.484   13.419  -220.823
247.773    3.495   -2.403
3.495   233.252   -4.285
-2.403   -4.285   245.876

orbtensor 14 C
-202.472   12.149  -10.569
12.149  -111.077  -37.099
-10.569  -37.099  -230.176
246.527  -0.617    4.642
-0.617  236.930    7.016
4.642    7.016   242.838

orbtensor 15 C
-56.470    0.997    6.681
0.997  -48.559    2.873
6.681    2.873  -50.088
219.885   -0.322    2.564
-0.322  218.624   -4.258
2.564   -4.258   228.708

orbtensor 16 H
2.962   -0.721    0.101
-0.721    1.912    1.407
0.101    1.407    1.266
23.784    0.874   -0.628
0.874   29.299   -6.778
-0.628   -6.778   29.501

orbtensor 17 H
3.054    0.384   -1.960
0.384    3.379    2.362
-1.960    2.362    2.605
30.497   -0.478    0.421
-0.478   20.916   -2.417
0.421   -2.417   29.051

orbtensor 18 H

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5.022	0.265	-0.055
0.265	3.316	2.180
-0.055	2.180	-1.453
21.577	-2.496	-0.447
-2.496	26.719	1.350
-0.447	1.350	30.585

orbtensor 19 C

-54.157	-0.468	-5.666
-0.468	-46.188	2.624
-5.666	2.624	-55.366
226.851	0.725	-6.853
0.725	218.951	-1.278
-6.853	-1.278	223.738

orbtensor 20 H

2.078	-0.616	1.178
-0.616	2.017	0.835
1.178	0.835	2.205
26.999	3.474	-4.146
3.474	28.744	-5.104
-4.146	-5.104	26.847

orbtensor 21 H

2.335	-1.557	2.987
-1.557	3.830	0.890
2.987	0.890	0.222
25.919	2.911	-3.047
2.911	25.013	3.340
-3.047	3.340	28.585

orbtensor 22 H

-1.384	-0.860	1.455
-0.860	2.919	1.122
1.455	1.122	3.523
33.936	-2.111	-0.718
-2.111	22.554	-1.227
-0.718	-1.227	26.121

orbtensor 23 C

-51.425	-0.852	4.722
-0.852	-46.581	-3.159
4.722	-3.159	-57.708
230.007	1.472	5.098
1.472	219.126	1.194
5.098	1.194	220.408

orbtensor 24 C

-59.344	-0.148	-4.210
-0.148	-48.965	-2.956
-4.210	-2.956	-46.792
219.178	0.770	-0.147
0.770	219.255	4.888
-0.147	4.888	228.779

orbtensor 25 H

2.820	-1.078	-0.422
-1.078	1.729	-1.201
-0.422	-1.201	1.589
24.415	2.648	1.722
2.648	30.204	6.255
1.722	6.255	27.964

orbtensor 26 H

4.631	-0.390	-1.507
-0.390	2.994	-2.463
-1.507	-2.463	-0.741

22.440	-2.614	2.801
-2.614	26.589	-0.430
2.801	-0.430	29.854

orbtensor 27 H

3.998	-0.114	1.628
-0.114	3.047	-2.462
1.628	-2.462	1.997
30.190	0.192	-0.759
0.192	21.289	2.998
-0.759	2.998	28.982

orbtensor 28 H

-5.777	-6.386	0.619
-6.386	-16.718	1.316
0.619	1.316	-2.851
32.096	5.149	-1.294
5.149	41.605	-1.299
-1.294	-1.299	23.732

orbtensor 29 H

-18.504	-2.662	2.281
-2.662	-3.478	0.409
2.281	0.409	-1.965
41.673	2.199	-2.712
2.199	30.611	-0.607
-2.712	-0.607	21.760

orbtensor 30 C

-235.404	-7.251	-10.039
-7.251	-96.936	-20.510
-10.039	-20.510	-211.983
248.756	4.705	1.279
4.705	233.828	4.010
1.279	4.010	244.323

orbtensor 31 H

-1.762	-1.159	0.030
-1.159	2.788	-0.790
0.030	-0.790	4.033
33.813	-1.714	-1.205
-1.714	22.772	1.950
-1.205	1.950	26.028

orbtensor 32 H

0.752	-1.966	-2.990
-1.966	3.723	-0.620
-2.990	-0.620	1.907
27.559	2.209	3.202
2.209	24.528	-3.781
3.202	-3.781	27.428

orbtensor 33 H

1.519	-0.878	-0.931
-0.878	1.917	-0.601
-0.931	-0.601	2.862
28.951	4.889	3.212
4.889	29.357	3.775
3.212	3.775	24.283

orbtensor 34 H

-8.215	3.713	0.856
3.713	-14.390	-0.003
0.856	-0.003	-0.751
34.829	-1.316	-1.911
-1.316	36.463	-0.411
-1.911	-0.411	20.016

orbtensor 35 H
 -18.329 0.609 2.094
 0.609 -3.406 -0.031
 2.094 -0.031 -2.308
 42.213 -0.596 -2.651
 -0.596 30.454 -0.230
 -2.651 -0.230 21.988

orbtensor 36 H
 -8.095 7.662 0.355
 7.662 -13.776 -0.629
 0.355 -0.629 -3.327
 34.069 -6.703 -1.154
 -6.703 38.535 0.341
 -1.154 0.341 23.515

orbtensor 37 H
 -5.360 -5.153 0.654
 -5.153 -16.460 1.184
 0.654 1.184 -1.827
 31.636 1.659 -1.305
 1.659 40.316 -0.852
 -1.305 -0.852 22.234

orbtensor 38 Cr
 -4995.561 438.282 -76.226
 438.282 -3640.003 -119.878
 -76.226 -119.878 -5452.191
 1814.620 1.011 -0.424
 1.011 1814.563 -0.233
 -0.424 -0.233 1811.689

orbtensor 39 Cl
 -322.415 -20.258 15.031
 -20.258 -460.519 164.382
 15.031 164.382 -394.034
 1141.122 -0.744 -2.553
 -0.744 1145.107 5.235
 -2.553 5.235 1146.575

orbtensor 40 Cl
 -333.399 -62.189 -25.241
 -62.189 -482.016 -147.288
 -25.241 -147.288 -361.469
 1142.777 -1.828 3.741
 -1.828 1144.418 -4.803
 3.741 -4.803 1145.611

gtensor (ppt)
 -0.152 0.005 -0.001
 0.005 -0.153 -0.001
 -0.001 -0.001 -0.154
 -3.907 3.399 -0.902
 3.399 -2.988 -0.682
 -0.902 -0.682 -9.807

zfstensor (cm-1)
 -0.433749 -0.170280 0.025825
 -0.170280 0.625406 0.050200
 0.025825 0.050200 -0.191656

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.2393	-37.05500	4093.17534	-3.20149	4089.97386	4052.91886

2	C	3.6023	25.37933	-1892.46595	-0.52309	-1892.98904	-1867.60971
3	C	-0.6890	57.55500	361.96235	-0.85383	361.10852	418.66352
4	C	1.2713	45.63167	-667.88796	0.55760	-667.33036	-621.69869
5	C	-1.1263	49.49833	591.71300	-0.30642	591.40658	640.90491
6	C	0.4670	23.35567	-245.33587	-0.43523	-245.77110	-222.41543
7	C	0.2437	53.48767	-128.00894	0.14109	-127.86785	-74.38018
8	C	-0.3647	53.28667	191.57562	-0.00527	191.57035	244.85702
9	C	-0.7590	48.33800	398.73646	0.50688	399.24334	447.58134
10	C	0.6087	42.74200	-319.75968	0.47814	-319.28154	-276.53954
11	C	-0.5263	54.71067	276.50631	0.62373	277.13004	331.84071
12	C	1.4093	60.84500	-740.38549	0.92605	-739.45944	-678.61444
13	C	1.1810	60.86567	-620.43184	-2.62631	-623.05814	-562.19248
14	C	1.4097	60.85667	-740.56061	1.42819	-739.13242	-678.27575
15	C	0.4917	170.70000	-258.29437	0.46432	-257.83005	-87.13005
16	H	1.0670	29.57467	-140.97860	0.17513	-140.80347	-111.22881
17	H	0.2030	29.83400	-26.82161	0.32813	-26.49348	3.34052
18	H	0.1217	28.58867	-16.07535	0.27754	-15.79781	12.79086
19	C	0.3563	171.27633	-187.19775	-0.81662	-188.01438	-16.73804
20	H	-0.5007	29.63000	66.15116	-0.31695	65.83421	95.46421
21	H	-0.1890	28.63467	24.97184	-0.44206	24.52978	53.16444
22	H	-0.0647	29.22300	8.54416	-0.74968	7.79448	37.01748
23	C	0.3560	171.27567	-187.02264	-0.76988	-187.79252	-16.51685
24	C	0.4937	170.70367	-259.34506	0.65877	-258.68629	-87.98262
25	H	1.0710	29.57367	-141.50711	0.25568	-141.25143	-111.67776
26	H	0.1220	28.58900	-16.11939	0.38662	-15.73277	12.85623
27	H	0.2043	29.83433	-26.99778	0.45311	-26.54466	3.28967
28	H	0.6680	24.02900	-88.26027	-0.32999	-88.59026	-64.56126
29	H	-1.4423	23.36567	190.56995	-0.40640	190.16355	213.52921
30	C	1.1793	60.86133	-619.55626	-2.46819	-622.02445	-561.16312
31	H	-0.0653	29.22400	8.63224	-0.73982	7.89243	37.11643
32	H	-0.1907	28.63233	25.19205	-0.41519	24.77686	53.40919
33	H	-0.5050	29.62967	66.72371	-0.28532	66.43839	96.06806
34	H	-1.6450	22.65067	217.34752	-0.68491	216.66260	239.31327
35	H	-0.4167	23.53733	55.05256	-0.06998	54.98258	78.51992
36	H	0.0897	23.64033	-11.84731	0.04282	-11.80450	11.83584
37	H	-0.2727	23.51300	36.02640	0.24180	36.26820	59.78120
38	Cr	23.9623	-2882.29433	55900.21911	-3.45770	55896.76141	53014.46708
39	Cl	1.3643	751.94533	-1837.69029	-12.10088	-1849.79117	-1097.84584
40	Cl	1.3633	751.97400	-1836.34334	-8.91287	-1845.25621	-1093.28221

=====
CrL1-STO-BP-ORCA
Temperature: 295
Spin: 1.5

atensor 1 N
-1.397 0.228 -0.236
0.228 -2.244 -0.061
-0.236 -0.061 -3.118
-0.011 0.030 0.003
-0.003 0.030 0.000
0.005 -0.004 0.022

atensor 2 C
2.752 0.953 0.423
0.953 1.883 0.029
0.423 0.029 6.211
-0.048 0.013 0.006
0.013 0.006 -0.002
0.006 -0.002 0.003

atensor 3 C
0.210 0.161 -0.276
0.161 -0.437 -0.071
-0.276 -0.071 -1.834
0.001 -0.009 0.000

0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C
0.125 0.072 0.533
0.072 -0.462 0.155
0.533 0.155 4.169
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.632 -0.093 -0.134
-0.093 -1.080 -0.009
-0.134 -0.009 -1.673
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.338 -0.515 -0.057
-0.515 -0.701 0.118
-0.057 0.118 0.770
0.007 0.000 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.114 -0.110 0.090
-0.110 -0.144 0.046
0.090 0.046 0.765
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.147 -0.154 -0.071
-0.154 -0.219 0.002
-0.071 0.002 -0.727
0.000 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.114 -0.245 0.131
-0.245 -0.968 0.060
0.131 0.060 -0.190
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.235 -0.950 -0.180
-0.950 0.978 0.076
-0.180 0.076 -0.382
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.004

atensor 11 C
0.213 -1.559 0.008
-1.559 -1.769 0.257
0.008 0.258 -0.149
0.059 0.019 0.002
-0.008 -0.015 0.004
0.003 0.001 0.082

atensor 12 C
0.227 -0.329 -0.008
-0.329 2.532 -2.301
-0.008 -2.301 1.365
0.060 0.000 0.000
-0.010 0.001 0.030
-0.008 0.027 0.043

atensor 13 C
1.911 1.560 -0.818
1.560 0.349 -1.040
-0.818 -1.041 1.168
0.039 -0.013 0.003
-0.029 0.011 0.021
0.005 0.018 0.065

atensor 14 C
0.300 0.267 0.250
0.267 2.845 2.207
0.250 2.207 0.980
0.061 -0.007 -0.004
-0.016 -0.003 -0.024
0.005 -0.023 0.046

atensor 15 C
-0.020 -0.220 0.287
-0.220 0.438 -0.792
0.287 -0.792 1.044
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.130 -0.140 0.191
-0.140 1.601 -1.417
0.191 -1.417 1.469
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.149 -1.225 1.523
-1.225 -0.004 -1.757
1.523 -1.757 0.761
0.003 0.004 -0.006
0.001 0.001 0.007
-0.007 0.012 -0.003

atensor 18 H
-1.740 -0.233 0.505
-0.233 -0.951 -1.805
0.505 -1.805 3.060
0.005 -0.003 -0.007
-0.003 0.008 0.004
0.000 0.013 -0.017

atensor 19 C
0.542 0.421 -0.618
0.421 0.072 -0.374
-0.618 -0.374 0.443
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.477 0.938 -0.868
0.938 -0.434 -0.862

-0.868 -0.862 -0.597
0.003 -0.003 0.000
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.224 0.814 -2.299
0.814 -1.531 -1.016
-2.299 -1.016 1.182
0.003 -0.003 0.006
0.001 0.009 -0.001
0.012 0.009 -0.006

atensor 22 H
1.624 1.099 -1.450
1.099 -1.082 -0.541
-1.450 -0.541 -0.747
0.000 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.831 0.542 0.476
0.542 0.116 0.260
0.476 0.260 0.109
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.090 -0.015 0.006
-0.015 0.554 0.861
0.006 0.861 1.004
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.123 0.222 0.137
0.222 1.799 1.386
0.137 1.386 1.290
0.002 0.001 0.003
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.680 0.277 0.712
0.277 -0.684 2.061
0.712 2.061 2.734
0.005 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.013 -0.016

atensor 27 H
-0.826 -0.818 -1.066
-0.818 0.261 2.083
-1.066 2.083 1.178
0.006 0.001 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.487 0.624 -0.222
0.624 0.535 -0.102
-0.222 -0.102 -0.021
0.000 -0.005 0.001
0.000 -0.001 0.000

0.000 0.001 0.004

atensor 29 H
-0.073 0.282 -0.224
0.282 -2.559 -0.008
-0.224 -0.008 -1.694
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.234 1.821 0.401
1.821 0.461 0.637
0.401 0.637 0.728
0.039 -0.017 0.005
-0.033 0.009 -0.009
0.004 -0.011 0.067

atensor 31 H
2.163 1.272 0.591
1.272 -1.028 0.230
0.591 0.230 -1.341
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.007

atensor 32 H
0.981 1.224 2.263
1.224 -1.401 0.887
2.263 0.887 -0.158
-0.002 -0.006 -0.006
0.000 0.009 0.000
-0.013 -0.008 -0.001

atensor 33 H
-0.081 1.176 0.643
1.176 -0.340 0.555
0.643 0.555 -1.100
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.378 2.944 -0.452
2.944 0.407 -0.539
-0.452 -0.539 -3.994
0.010 -0.001 0.002
-0.009 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.192 -0.289 -0.111
-0.289 -0.720 0.037
-0.111 0.037 -0.723
-0.001 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.337 -0.372 -0.060
-0.372 0.152 0.035
-0.060 0.035 -0.219
-0.001 0.002 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H

-0.558 -0.586 -0.010
-0.586 0.537 0.030
-0.010 0.030 -0.794
-0.002 0.001 0.000
0.002 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.863 2.936 -0.258
2.936 27.658 -0.725
-0.258 -0.725 17.715
2.429 -0.364 0.113
-0.384 2.040 0.090
0.113 0.087 3.182

atensor 39 Cl
6.351 0.146 1.824
0.146 2.731 -4.905
1.824 -4.905 -6.066
0.474 0.039 0.038
0.036 0.256 -0.190
0.006 -0.267 0.347

atensor 40 Cl
4.614 1.091 -4.778
1.091 3.350 4.144
-4.778 4.144 -4.950
0.453 0.102 -0.075
0.082 0.286 0.180
-0.042 0.254 0.337

orbtensor 1 N
-476.767 51.958 48.516
51.958 -551.690 9.313
48.516 9.313 -96.157
338.521 -2.790 -2.014
-2.790 352.359 -0.683
-2.014 -0.683 322.569

orbtensor 2 C
-269.772 25.851 25.162
25.851 -298.646 4.626
25.162 4.626 -72.625
253.092 6.157 -5.665
6.157 252.127 -2.226
-5.665 -2.226 211.962

orbtensor 3 C
-222.771 -47.342 23.622
-47.342 -286.652 14.261
23.622 14.261 -57.225
252.337 3.889 -3.913
3.889 263.144 -1.894
-3.913 -1.894 223.832

orbtensor 4 C
-301.509 -22.132 32.894
-22.132 -231.418 9.044
32.894 9.044 -58.839
257.133 3.287 -5.268
3.287 253.321 -1.676
-5.268 -1.676 218.207

orbtensor 5 C
-287.597 2.684 30.137
2.684 -276.312 7.364
30.137 7.364 -59.009

269.078	0.621	-4.475
0.621	266.926	-1.201
-4.475	-1.201	235.409

orbtensor 6 C

-273.672	19.767	22.021
19.767	-298.093	4.353
22.021	4.353	-101.825
263.297	-4.674	-5.740
-4.674	261.723	-0.917
-5.740	-0.917	218.637

orbtensor 7 C

-295.829	12.610	30.563
12.610	-210.969	3.731
30.563	3.731	-61.195
257.851	-4.101	-5.085
-4.101	252.330	-0.679
-5.085	-0.679	218.275

orbtensor 8 C

-247.413	53.705	24.004
53.705	-272.020	0.832
24.004	0.832	-51.239
253.687	-5.371	-4.182
-5.371	256.250	-0.566
-4.182	-0.566	220.595

orbtensor 9 C

-236.953	-36.098	24.846
-36.098	-289.836	12.853
24.846	12.853	-58.877
253.125	-3.421	-4.280
-3.421	257.730	-0.897
-4.280	-0.897	219.825

orbtensor 10 C

-302.885	-14.652	28.573
-14.652	-250.073	7.595
28.573	7.595	-90.683
270.314	-0.813	-4.470
-0.813	265.280	-0.927
-4.470	-0.927	236.273

orbtensor 11 C

-220.827	33.177	0.122
33.177	-134.300	-6.951
0.122	-6.951	-210.845
250.310	-7.752	-1.266
-7.752	241.165	0.911
-1.266	0.911	238.629

orbtensor 12 C

-199.453	20.524	0.690
20.524	-106.842	24.199
0.690	24.199	-237.466
244.041	-2.650	-4.723
-2.650	236.024	-6.038
-4.723	-6.038	246.231

orbtensor 13 C

-228.891	-1.967	14.484
-1.967	-94.590	13.419
14.484	13.419	-220.823
247.773	3.495	-2.403
3.495	233.252	-4.285
-2.403	-4.285	245.876

orbtensor 14 C
-202.472 12.149 -10.569
12.149 -111.077 -37.099
-10.569 -37.099 -230.176
246.527 -0.617 4.642
-0.617 236.930 7.016
4.642 7.016 242.838

orbtensor 15 C
-56.470 0.997 6.681
0.997 -48.559 2.873
6.681 2.873 -50.088
219.885 -0.322 2.564
-0.322 218.624 -4.258
2.564 -4.258 228.708

orbtensor 16 H
2.962 -0.721 0.101
-0.721 1.912 1.407
0.101 1.407 1.266
23.784 0.874 -0.628
0.874 29.299 -6.778
-0.628 -6.778 29.501

orbtensor 17 H
3.054 0.384 -1.960
0.384 3.379 2.362
-1.960 2.362 2.605
30.497 -0.478 0.421
-0.478 20.916 -2.417
0.421 -2.417 29.051

orbtensor 18 H
5.022 0.265 -0.055
0.265 3.316 2.180
-0.055 2.180 -1.453
21.577 -2.496 -0.447
-2.496 26.719 1.350
-0.447 1.350 30.585

orbtensor 19 C
-54.157 -0.468 -5.666
-0.468 -46.188 2.624
-5.666 2.624 -55.366
226.851 0.725 -6.853
0.725 218.951 -1.278
-6.853 -1.278 223.738

orbtensor 20 H
2.078 -0.616 1.178
-0.616 2.017 0.835
1.178 0.835 2.205
26.999 3.474 -4.146
3.474 28.744 -5.104
-4.146 -5.104 26.847

orbtensor 21 H
2.335 -1.557 2.987
-1.557 3.830 0.890
2.987 0.890 0.222
25.919 2.911 -3.047
2.911 25.013 3.340
-3.047 3.340 28.585

orbtensor 22 H
-1.384 -0.860 1.455

-0.860	2.919	1.122
1.455	1.122	3.523
33.936	-2.111	-0.718
-2.111	22.554	-1.227
-0.718	-1.227	26.121

orbtensor 23 C

-51.425	-0.852	4.722
-0.852	-46.581	-3.159
4.722	-3.159	-57.708
230.007	1.472	5.098
1.472	219.126	1.194
5.098	1.194	220.408

orbtensor 24 C

-59.344	-0.148	-4.210
-0.148	-48.965	-2.956
-4.210	-2.956	-46.792
219.178	0.770	-0.147
0.770	219.255	4.888
-0.147	4.888	228.779

orbtensor 25 H

2.820	-1.078	-0.422
-1.078	1.729	-1.201
-0.422	-1.201	1.589
24.415	2.648	1.722
2.648	30.204	6.255
1.722	6.255	27.964

orbtensor 26 H

4.631	-0.390	-1.507
-0.390	2.994	-2.463
-1.507	-2.463	-0.741
22.440	-2.614	2.801
-2.614	26.589	-0.430
2.801	-0.430	29.854

orbtensor 27 H

3.998	-0.114	1.628
-0.114	3.047	-2.462
1.628	-2.462	1.997
30.190	0.192	-0.759
0.192	21.289	2.998
-0.759	2.998	28.982

orbtensor 28 H

-5.777	-6.386	0.619
-6.386	-16.718	1.316
0.619	1.316	-2.851
32.096	5.149	-1.294
5.149	41.605	-1.299
-1.294	-1.299	23.732

orbtensor 29 H

-18.504	-2.662	2.281
-2.662	-3.478	0.409
2.281	0.409	-1.965
41.673	2.199	-2.712
2.199	30.611	-0.607
-2.712	-0.607	21.760

orbtensor 30 C

-235.404	-7.251	-10.039
-7.251	-96.936	-20.510
-10.039	-20.510	-211.983
248.756	4.705	1.279

4.705 233.828 4.010
1.279 4.010 244.323

orbtensor 31 H
-1.762 -1.159 0.030
-1.159 2.788 -0.790
0.030 -0.790 4.033
33.813 -1.714 -1.205
-1.714 22.772 1.950
-1.205 1.950 26.028

orbtensor 32 H
0.752 -1.966 -2.990
-1.966 3.723 -0.620
-2.990 -0.620 1.907
27.559 2.209 3.202
2.209 24.528 -3.781
3.202 -3.781 27.428

orbtensor 33 H
1.519 -0.878 -0.931
-0.878 1.917 -0.601
-0.931 -0.601 2.862
28.951 4.889 3.212
4.889 29.357 3.775
3.212 3.775 24.283

orbtensor 34 H
-8.215 3.713 0.856
3.713 -14.390 -0.003
0.856 -0.003 -0.751
34.829 -1.316 -1.911
-1.316 36.463 -0.411
-1.911 -0.411 20.016

orbtensor 35 H
-18.329 0.609 2.094
0.609 -3.406 -0.031
2.094 -0.031 -2.308
42.213 -0.596 -2.651
-0.596 30.454 -0.230
-2.651 -0.230 21.988

orbtensor 36 H
-8.095 7.662 0.355
7.662 -13.776 -0.629
0.355 -0.629 -3.327
34.069 -6.703 -1.154
-6.703 38.535 0.341
-1.154 0.341 23.515

orbtensor 37 H
-5.360 -5.153 0.654
-5.153 -16.460 1.184
0.654 1.184 -1.827
31.636 1.659 -1.305
1.659 40.316 -0.852
-1.305 -0.852 22.234

orbtensor 38 Cr
-4995.561 438.282 -76.226
438.282 -3640.003 -119.878
-76.226 -119.878 -5452.191
1814.620 1.011 -0.424
1.011 1814.563 -0.233
-0.424 -0.233 1811.689

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orbtensor 39 C1
-322.415  -20.258   15.031
-20.258  -460.519  164.382
15.031   164.382 -394.034
1141.122  -0.744   -2.553
-0.744   1145.107  5.235
-2.553    5.235  1146.575

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orbtensor 40 C1
-333.399  -62.189  -25.241
-62.189  -482.016 -147.288
-25.241  -147.288 -361.469
1142.777  -1.828   3.741
-1.828   1144.418  -4.803
3.741    -4.803  1145.611

```

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gtensor (ppt)
-0.152    0.005   -0.001
0.005   -0.153   -0.001
-0.001   -0.001   -0.154
-3.907    3.399   -0.902
3.399   -2.988   -0.682
-0.902   -0.682   -9.807

```

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zfstensor (cm-1)
-1.018591  0.216678   0.027448
 0.216678  0.243991  -0.062538
 0.027448 -0.062538  -0.753365

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.2393	-37.05500	4093.16263	-2.54355	4090.61907	4053.56407
2	C	3.6023	25.37933	-1892.46007	-0.06251	-1892.52258	-1867.14324
3	C	-0.6890	57.55500	361.96123	-0.69073	361.27050	418.82550
4	C	1.2713	45.63167	-667.88588	0.28893	-667.59695	-621.96528
5	C	-1.1263	49.49833	591.71117	-0.38099	591.33018	640.82851
6	C	0.4670	23.35567	-245.33511	-1.11236	-246.44747	-223.09180
7	C	0.2437	53.48767	-128.00854	-0.02419	-128.03273	-74.54507
8	C	-0.3647	53.28667	191.57503	-0.10298	191.47204	244.75871
9	C	-0.7590	48.33800	398.73523	0.26841	399.00363	447.34163
10	C	0.6087	42.74200	-319.75868	-0.23422	-319.99291	-277.25091
11	C	-0.5263	54.71067	276.50545	-0.90637	275.59908	330.30975
12	C	1.4093	60.84500	-740.38319	1.41572	-738.96748	-678.12248
13	C	1.1810	60.86567	-620.42991	-1.35366	-621.78357	-560.91790
14	C	1.4097	60.85667	-740.55831	1.41726	-739.14105	-678.28438
15	C	0.4917	170.70000	-258.29357	0.47340	-257.82017	-87.12017
16	H	1.0670	29.57467	-140.97816	0.25911	-140.71905	-111.14438
17	H	0.2030	29.83400	-26.82153	0.18066	-26.64087	3.19313
18	H	0.1217	28.58867	-16.07530	0.29624	-15.77906	12.80961
19	C	0.3563	171.27633	-187.19717	-0.46112	-187.65829	-16.38196
20	H	-0.5007	29.63000	66.15095	-0.08020	66.07076	95.70076
21	H	-0.1890	28.63467	24.97176	-0.28619	24.68558	53.32025
22	H	-0.0647	29.22300	8.54413	-0.55976	7.98437	37.20737
23	C	0.3560	171.27567	-187.02206	-0.45930	-187.48135	-16.20569
24	C	0.4937	170.70367	-259.34425	0.47343	-258.87083	-88.16716
25	H	1.0710	29.57367	-141.50667	0.25927	-141.24740	-111.67373
26	H	0.1220	28.58900	-16.11934	0.29632	-15.82302	12.76598
27	H	0.2043	29.83433	-26.99769	0.17985	-26.81785	3.01649
28	H	0.6680	24.02900	-88.25999	-0.21237	-88.47236	-64.44336
29	H	-1.4423	23.36567	190.56936	-0.40979	190.15957	213.52524
30	C	1.1793	60.86133	-619.55434	-1.35395	-620.90829	-560.04696
31	H	-0.0653	29.22400	8.63221	-0.55907	8.07314	37.29714
32	H	-0.1907	28.63233	25.19197	-0.28514	24.90683	53.53916
33	H	-0.5050	29.62967	66.72350	-0.07963	66.64387	96.27354
34	H	-1.6450	22.65067	217.34684	0.01982	217.36666	240.01733

35	H	-0.4167	23.53733	55.05239	-0.14667	54.90573	78.44306
36	H	0.0897	23.64033	-11.84727	-0.03109	-11.87837	11.76197
37	H	-0.2727	23.51300	36.02628	0.16342	36.18971	59.70271
38	Cr	23.9623	-2882.29433	55900.04543	-17.99677	55882.04866	52999.75433
39	Cl	1.3643	751.94533	-1837.68458	-8.26263	-1845.94721	-1094.00188
40	Cl	1.3633	751.97400	-1836.33763	-8.27327	-1844.61090	-1092.63690

=====
CrL1-STO-BP-Pederson

Temperature: 295

Spin: 1.5

atensor 1 N

-1.397 0.228 -0.236
0.228 -2.244 -0.061
-0.236 -0.061 -3.118
-0.011 0.030 0.003
-0.003 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.752 0.953 0.423
0.953 1.883 0.029
0.423 0.029 6.211
-0.048 0.013 0.006
0.013 0.006 -0.002
0.006 -0.002 0.003

atensor 3 C

0.210 0.161 -0.276
0.161 -0.437 -0.071
-0.276 -0.071 -1.834
0.001 -0.009 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C

0.125 0.072 0.533
0.072 -0.462 0.155
0.533 0.155 4.169
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C

-0.632 -0.093 -0.134
-0.093 -1.080 -0.009
-0.134 -0.009 -1.673
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C

1.338 -0.515 -0.057
-0.515 -0.701 0.118
-0.057 0.118 0.770
0.007 0.000 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C

0.114 -0.110 0.090
-0.110 -0.144 0.046
0.090 0.046 0.765
0.000 0.002 0.000
-0.001 -0.004 0.000

0.000 0.000 0.000

atensor 8 C

-0.147 -0.154 -0.071
-0.154 -0.219 0.002
-0.071 0.002 -0.727
0.000 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C

-1.114 -0.245 0.131
-0.245 -0.968 0.060
0.131 0.060 -0.190
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C

1.235 -0.950 -0.180
-0.950 0.978 0.076
-0.180 0.076 -0.382
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.004

atensor 11 C

0.213 -1.559 0.008
-1.559 -1.769 0.257
0.008 0.258 -0.149
0.059 0.019 0.002
-0.008 -0.015 0.004
0.003 0.001 0.082

atensor 12 C

0.227 -0.329 -0.008
-0.329 2.532 -2.301
-0.008 -2.301 1.365
0.060 0.000 0.000
-0.010 0.001 0.030
-0.008 0.027 0.043

atensor 13 C

1.911 1.560 -0.818
1.560 0.349 -1.040
-0.818 -1.041 1.168
0.039 -0.013 0.003
-0.029 0.011 0.021
0.005 0.018 0.065

atensor 14 C

0.300 0.267 0.250
0.267 2.845 2.207
0.250 2.207 0.980
0.061 -0.007 -0.004
-0.016 -0.003 -0.024
0.005 -0.023 0.046

atensor 15 C

-0.020 -0.220 0.287
-0.220 0.438 -0.792
0.287 -0.792 1.044
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H

0.130 -0.140 0.191
-0.140 1.601 -1.417
0.191 -1.417 1.469
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.149 -1.225 1.523
-1.225 -0.004 -1.757
1.523 -1.757 0.761
0.003 0.004 -0.006
0.001 0.001 0.007
-0.007 0.012 -0.003

atensor 18 H
-1.740 -0.233 0.505
-0.233 -0.951 -1.805
0.505 -1.805 3.060
0.005 -0.003 -0.007
-0.003 0.008 0.004
0.000 0.013 -0.017

atensor 19 C
0.542 0.421 -0.618
0.421 0.072 -0.374
-0.618 -0.374 0.443
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.477 0.938 -0.868
0.938 -0.434 -0.862
-0.868 -0.862 -0.597
0.003 -0.003 0.000
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.224 0.814 -2.299
0.814 -1.531 -1.016
-2.299 -1.016 1.182
0.003 -0.003 0.006
0.001 0.009 -0.001
0.012 0.009 -0.006

atensor 22 H
1.624 1.099 -1.450
1.099 -1.082 -0.541
-1.450 -0.541 -0.747
0.000 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.831 0.542 0.476
0.542 0.116 0.260
0.476 0.260 0.109
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.090 -0.015 0.006
-0.015 0.554 0.861
0.006 0.861 1.004

0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.123 0.222 0.137
0.222 1.799 1.386
0.137 1.386 1.290
0.002 0.001 0.003
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.680 0.277 0.712
0.277 -0.684 2.061
0.712 2.061 2.734
0.005 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.013 -0.016

atensor 27 H
-0.826 -0.818 -1.066
-0.818 0.261 2.083
-1.066 2.083 1.178
0.006 0.001 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.487 0.624 -0.222
0.624 0.535 -0.102
-0.222 -0.102 -0.021
0.000 -0.005 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
-0.073 0.282 -0.224
0.282 -2.559 -0.008
-0.224 -0.008 -1.694
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.234 1.821 0.401
1.821 0.461 0.637
0.401 0.637 0.728
0.039 -0.017 0.005
-0.033 0.009 -0.009
0.004 -0.011 0.067

atensor 31 H
2.163 1.272 0.591
1.272 -1.028 0.230
0.591 0.230 -1.341
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.007

atensor 32 H
0.981 1.224 2.263
1.224 -1.401 0.887
2.263 0.887 -0.158
-0.002 -0.006 -0.006
0.000 0.009 0.000
-0.013 -0.008 -0.001

atensor 33 H
-0.081 1.176 0.643
1.176 -0.340 0.555
0.643 0.555 -1.100
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.378 2.944 -0.452
2.944 0.407 -0.539
-0.452 -0.539 -3.994
0.010 -0.001 0.002
-0.009 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.192 -0.289 -0.111
-0.289 -0.720 0.037
-0.111 0.037 -0.723
-0.001 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.337 -0.372 -0.060
-0.372 0.152 0.035
-0.060 0.035 -0.219
-0.001 0.002 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.558 -0.586 -0.010
-0.586 0.537 0.030
-0.010 0.030 -0.794
-0.002 0.001 0.000
0.002 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.863 2.936 -0.258
2.936 27.658 -0.725
-0.258 -0.725 17.715
2.429 -0.364 0.113
-0.384 2.040 0.090
0.113 0.087 3.182

atensor 39 Cl
6.351 0.146 1.824
0.146 2.731 -4.905
1.824 -4.905 -6.066
0.474 0.039 0.038
0.036 0.256 -0.190
0.006 -0.267 0.347

atensor 40 Cl
4.614 1.091 -4.778
1.091 3.350 4.144
-4.778 4.144 -4.950
0.453 0.102 -0.075
0.082 0.286 0.180
-0.042 0.254 0.337

orbtensor 1 N
-476.767 51.958 48.516

51.958	-551.690	9.313
48.516	9.313	-96.157
338.521	-2.790	-2.014
-2.790	352.359	-0.683
-2.014	-0.683	322.569

orbtensor 2 C

-269.772	25.851	25.162
25.851	-298.646	4.626
25.162	4.626	-72.625
253.092	6.157	-5.665
6.157	252.127	-2.226
-5.665	-2.226	211.962

orbtensor 3 C

-222.771	-47.342	23.622
-47.342	-286.652	14.261
23.622	14.261	-57.225
252.337	3.889	-3.913
3.889	263.144	-1.894
-3.913	-1.894	223.832

orbtensor 4 C

-301.509	-22.132	32.894
-22.132	-231.418	9.044
32.894	9.044	-58.839
257.133	3.287	-5.268
3.287	253.321	-1.676
-5.268	-1.676	218.207

orbtensor 5 C

-287.597	2.684	30.137
2.684	-276.312	7.364
30.137	7.364	-59.009
269.078	0.621	-4.475
0.621	266.926	-1.201
-4.475	-1.201	235.409

orbtensor 6 C

-273.672	19.767	22.021
19.767	-298.093	4.353
22.021	4.353	-101.825
263.297	-4.674	-5.740
-4.674	261.723	-0.917
-5.740	-0.917	218.637

orbtensor 7 C

-295.829	12.610	30.563
12.610	-210.969	3.731
30.563	3.731	-61.195
257.851	-4.101	-5.085
-4.101	252.330	-0.679
-5.085	-0.679	218.275

orbtensor 8 C

-247.413	53.705	24.004
53.705	-272.020	0.832
24.004	0.832	-51.239
253.687	-5.371	-4.182
-5.371	256.250	-0.566
-4.182	-0.566	220.595

orbtensor 9 C

-236.953	-36.098	24.846
-36.098	-289.836	12.853
24.846	12.853	-58.877
253.125	-3.421	-4.280

-3.421 257.730 -0.897
-4.280 -0.897 219.825

orbtensor 10 C
-302.885 -14.652 28.573
-14.652 -250.073 7.595
28.573 7.595 -90.683
270.314 -0.813 -4.470
-0.813 265.280 -0.927
-4.470 -0.927 236.273

orbtensor 11 C
-220.827 33.177 0.122
33.177 -134.300 -6.951
0.122 -6.951 -210.845
250.310 -7.752 -1.266
-7.752 241.165 0.911
-1.266 0.911 238.629

orbtensor 12 C
-199.453 20.524 0.690
20.524 -106.842 24.199
0.690 24.199 -237.466
244.041 -2.650 -4.723
-2.650 236.024 -6.038
-4.723 -6.038 246.231

orbtensor 13 C
-228.891 -1.967 14.484
-1.967 -94.590 13.419
14.484 13.419 -220.823
247.773 3.495 -2.403
3.495 233.252 -4.285
-2.403 -4.285 245.876

orbtensor 14 C
-202.472 12.149 -10.569
12.149 -111.077 -37.099
-10.569 -37.099 -230.176
246.527 -0.617 4.642
-0.617 236.930 7.016
4.642 7.016 242.838

orbtensor 15 C
-56.470 0.997 6.681
0.997 -48.559 2.873
6.681 2.873 -50.088
219.885 -0.322 2.564
-0.322 218.624 -4.258
2.564 -4.258 228.708

orbtensor 16 H
2.962 -0.721 0.101
-0.721 1.912 1.407
0.101 1.407 1.266
23.784 0.874 -0.628
0.874 29.299 -6.778
-0.628 -6.778 29.501

orbtensor 17 H
3.054 0.384 -1.960
0.384 3.379 2.362
-1.960 2.362 2.605
30.497 -0.478 0.421
-0.478 20.916 -2.417
0.421 -2.417 29.051

orbtensor 18 H
5.022 0.265 -0.055
0.265 3.316 2.180
-0.055 2.180 -1.453
21.577 -2.496 -0.447
-2.496 26.719 1.350
-0.447 1.350 30.585

orbtensor 19 C
-54.157 -0.468 -5.666
-0.468 -46.188 2.624
-5.666 2.624 -55.366
226.851 0.725 -6.853
0.725 218.951 -1.278
-6.853 -1.278 223.738

orbtensor 20 H
2.078 -0.616 1.178
-0.616 2.017 0.835
1.178 0.835 2.205
26.999 3.474 -4.146
3.474 28.744 -5.104
-4.146 -5.104 26.847

orbtensor 21 H
2.335 -1.557 2.987
-1.557 3.830 0.890
2.987 0.890 0.222
25.919 2.911 -3.047
2.911 25.013 3.340
-3.047 3.340 28.585

orbtensor 22 H
-1.384 -0.860 1.455
-0.860 2.919 1.122
1.455 1.122 3.523
33.936 -2.111 -0.718
-2.111 22.554 -1.227
-0.718 -1.227 26.121

orbtensor 23 C
-51.425 -0.852 4.722
-0.852 -46.581 -3.159
4.722 -3.159 -57.708
230.007 1.472 5.098
1.472 219.126 1.194
5.098 1.194 220.408

orbtensor 24 C
-59.344 -0.148 -4.210
-0.148 -48.965 -2.956
-4.210 -2.956 -46.792
219.178 0.770 -0.147
0.770 219.255 4.888
-0.147 4.888 228.779

orbtensor 25 H
2.820 -1.078 -0.422
-1.078 1.729 -1.201
-0.422 -1.201 1.589
24.415 2.648 1.722
2.648 30.204 6.255
1.722 6.255 27.964

orbtensor 26 H
4.631 -0.390 -1.507
-0.390 2.994 -2.463

-1.507	-2.463	-0.741
22.440	-2.614	2.801
-2.614	26.589	-0.430
2.801	-0.430	29.854

orbtensor 27 H

3.998	-0.114	1.628
-0.114	3.047	-2.462
1.628	-2.462	1.997
30.190	0.192	-0.759
0.192	21.289	2.998
-0.759	2.998	28.982

orbtensor 28 H

-5.777	-6.386	0.619
-6.386	-16.718	1.316
0.619	1.316	-2.851
32.096	5.149	-1.294
5.149	41.605	-1.299
-1.294	-1.299	23.732

orbtensor 29 H

-18.504	-2.662	2.281
-2.662	-3.478	0.409
2.281	0.409	-1.965
41.673	2.199	-2.712
2.199	30.611	-0.607
-2.712	-0.607	21.760

orbtensor 30 C

-235.404	-7.251	-10.039
-7.251	-96.936	-20.510
-10.039	-20.510	-211.983
248.756	4.705	1.279
4.705	233.828	4.010
1.279	4.010	244.323

orbtensor 31 H

-1.762	-1.159	0.030
-1.159	2.788	-0.790
0.030	-0.790	4.033
33.813	-1.714	-1.205
-1.714	22.772	1.950
-1.205	1.950	26.028

orbtensor 32 H

0.752	-1.966	-2.990
-1.966	3.723	-0.620
-2.990	-0.620	1.907
27.559	2.209	3.202
2.209	24.528	-3.781
3.202	-3.781	27.428

orbtensor 33 H

1.519	-0.878	-0.931
-0.878	1.917	-0.601
-0.931	-0.601	2.862
28.951	4.889	3.212
4.889	29.357	3.775
3.212	3.775	24.283

orbtensor 34 H

-8.215	3.713	0.856
3.713	-14.390	-0.003
0.856	-0.003	-0.751
34.829	-1.316	-1.911
-1.316	36.463	-0.411

-1.911 -0.411 20.016

orbtensor 35 H

-18.329 0.609 2.094
0.609 -3.406 -0.031
2.094 -0.031 -2.308
42.213 -0.596 -2.651
-0.596 30.454 -0.230
-2.651 -0.230 21.988

orbtensor 36 H

-8.095 7.662 0.355
7.662 -13.776 -0.629
0.355 -0.629 -3.327
34.069 -6.703 -1.154
-6.703 38.535 0.341
-1.154 0.341 23.515

orbtensor 37 H

-5.360 -5.153 0.654
-5.153 -16.460 1.184
0.654 1.184 -1.827
31.636 1.659 -1.305
1.659 40.316 -0.852
-1.305 -0.852 22.234

orbtensor 38 Cr

-4995.561 438.282 -76.226
438.282 -3640.003 -119.878
-76.226 -119.878 -5452.191
1814.620 1.011 -0.424
1.011 1814.563 -0.233
-0.424 -0.233 1811.689

orbtensor 39 Cl

-322.415 -20.258 15.031
-20.258 -460.519 164.382
15.031 164.382 -394.034
1141.122 -0.744 -2.553
-0.744 1145.107 5.235
-2.553 5.235 1146.575

orbtensor 40 Cl

-333.399 -62.189 -25.241
-62.189 -482.016 -147.288
-25.241 -147.288 -361.469
1142.777 -1.828 3.741
-1.828 1144.418 -4.803
3.741 -4.803 1145.611

gtensor (ppt)

-0.152 0.005 -0.001
0.005 -0.153 -0.001
-0.001 -0.001 -0.154
-3.907 3.399 -0.902
3.399 -2.988 -0.682
-0.902 -0.682 -9.807

zfstensor (cm-1)

-0.237390 -0.152894 -0.008756
-0.152894 0.498855 0.046138
-0.008756 0.046138 -0.261466

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
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1	N	-2.2393	-37.05500	4093.17343	-2.33714	4090.83630	4053.78130
2	C	3.6023	25.37933	-1892.46507	-0.66267	-1893.12773	-1867.74840
3	C	-0.6890	57.55500	361.96218	-0.59933	361.36285	418.91785
4	C	1.2713	45.63167	-667.88764	0.31026	-667.57739	-621.94572
5	C	-1.1263	49.49833	591.71273	-0.17002	591.54271	641.04104
6	C	0.4670	23.35567	-245.33576	-0.14524	-245.48100	-222.12533
7	C	0.2437	53.48767	-128.00888	0.11815	-127.89073	-74.40306
8	C	-0.3647	53.28667	191.57553	0.04476	191.62030	244.90696
9	C	-0.7590	48.33800	398.73628	0.40184	399.13812	447.47612
10	C	0.6087	42.74200	-319.75953	0.60478	-319.15474	-276.41274
11	C	-0.5263	54.71067	276.50618	0.85417	277.36035	332.07102
12	C	1.4093	60.84500	-740.38515	0.56562	-739.81953	-678.97453
13	C	1.1810	60.86567	-620.43155	-2.25100	-622.68255	-561.81688
14	C	1.4097	60.85667	-740.56026	1.03556	-739.52471	-678.66804
15	C	0.4917	170.70000	-258.29425	0.31089	-257.98336	-87.28336
16	H	1.0670	29.57467	-140.97854	0.10218	-140.87636	-111.30169
17	H	0.2030	29.83400	-26.82160	0.27337	-26.54823	3.28577
18	H	0.1217	28.58867	-16.07534	0.15968	-15.91566	12.67300
19	C	0.3563	171.27633	-187.19766	-0.68789	-187.88555	-16.60922
20	H	-0.5007	29.63000	66.15113	-0.29070	65.86043	95.49043
21	H	-0.1890	28.63467	24.97183	-0.37506	24.59677	53.23143
22	H	-0.0647	29.22300	8.54415	-0.58388	7.96028	37.18328
23	C	0.3560	171.27567	-187.02255	-0.64346	-187.66601	-16.39034
24	C	0.4937	170.70367	-259.34494	0.49269	-258.85225	-88.14859
25	H	1.0710	29.57367	-141.50704	0.17753	-141.32951	-111.75584
26	H	0.1220	28.58900	-16.11938	0.26182	-15.85756	12.73144
27	H	0.2043	29.83433	-26.99776	0.38988	-26.60789	3.22645
28	H	0.6680	24.02900	-88.26023	-0.26275	-88.52297	-64.49397
29	H	-1.4423	23.36567	190.56986	-0.29095	190.27891	213.64457
30	C	1.1793	60.86133	-619.55597	-2.10172	-621.65770	-560.79636
31	H	-0.0653	29.22400	8.63224	-0.57427	8.05797	37.28197
32	H	-0.1907	28.63233	25.19204	-0.34898	24.84306	53.47539
33	H	-0.5050	29.62967	66.72367	-0.26082	66.46285	96.09252
34	H	-1.6450	22.65067	217.34741	-0.66066	216.68676	239.33743
35	H	-0.4167	23.53733	55.05254	-0.02497	55.02756	78.56490
36	H	0.0897	23.64033	-11.84731	0.05634	-11.79097	11.84937
37	H	-0.2727	23.51300	36.02638	0.20545	36.23183	59.74483
38	Cr	23.9623	-2882.29433	55900.19304	0.74707	55900.94010	53018.64577
39	Cl	1.3643	751.94533	-1837.68943	-8.76731	-1846.45674	-1094.51141
40	Cl	1.3633	751.97400	-1836.34248	-5.79945	-1842.14194	-1090.16794

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CrL1-STO-BP-Van-Wullen

Temperature: 295

Spin: 1.5

atensor 1 N

-1.397 0.228 -0.236
0.228 -2.244 -0.061
-0.236 -0.061 -3.118
-0.011 0.030 0.003
-0.003 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.752 0.953 0.423
0.953 1.883 0.029
0.423 0.029 6.211
-0.048 0.013 0.006
0.013 0.006 -0.002
0.006 -0.002 0.003

atensor 3 C

0.210 0.161 -0.276
0.161 -0.437 -0.071
-0.276 -0.071 -1.834

0.001 -0.009 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C
0.125 0.072 0.533
0.072 -0.462 0.155
0.533 0.155 4.169
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.632 -0.093 -0.134
-0.093 -1.080 -0.009
-0.134 -0.009 -1.673
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.338 -0.515 -0.057
-0.515 -0.701 0.118
-0.057 0.118 0.770
0.007 0.000 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.114 -0.110 0.090
-0.110 -0.144 0.046
0.090 0.046 0.765
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.147 -0.154 -0.071
-0.154 -0.219 0.002
-0.071 0.002 -0.727
0.000 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.114 -0.245 0.131
-0.245 -0.968 0.060
0.131 0.060 -0.190
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.235 -0.950 -0.180
-0.950 0.978 0.076
-0.180 0.076 -0.382
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.004

atensor 11 C
0.213 -1.559 0.008
-1.559 -1.769 0.257
0.008 0.258 -0.149
0.059 0.019 0.002
-0.008 -0.015 0.004
0.003 0.001 0.082

atensor 12 C
0.227 -0.329 -0.008
-0.329 2.532 -2.301
-0.008 -2.301 1.365
0.060 0.000 0.000
-0.010 0.001 0.030
-0.008 0.027 0.043

atensor 13 C
1.911 1.560 -0.818
1.560 0.349 -1.040
-0.818 -1.041 1.168
0.039 -0.013 0.003
-0.029 0.011 0.021
0.005 0.018 0.065

atensor 14 C
0.300 0.267 0.250
0.267 2.845 2.207
0.250 2.207 0.980
0.061 -0.007 -0.004
-0.016 -0.003 -0.024
0.005 -0.023 0.046

atensor 15 C
-0.020 -0.220 0.287
-0.220 0.438 -0.792
0.287 -0.792 1.044
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.130 -0.140 0.191
-0.140 1.601 -1.417
0.191 -1.417 1.469
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.149 -1.225 1.523
-1.225 -0.004 -1.757
1.523 -1.757 0.761
0.003 0.004 -0.006
0.001 0.001 0.007
-0.007 0.012 -0.003

atensor 18 H
-1.740 -0.233 0.505
-0.233 -0.951 -1.805
0.505 -1.805 3.060
0.005 -0.003 -0.007
-0.003 0.008 0.004
0.000 0.013 -0.017

atensor 19 C
0.542 0.421 -0.618
0.421 0.072 -0.374
-0.618 -0.374 0.443
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.477 0.938 -0.868

0.938 -0.434 -0.862
-0.868 -0.862 -0.597
0.003 -0.003 0.000
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.224 0.814 -2.299
0.814 -1.531 -1.016
-2.299 -1.016 1.182
0.003 -0.003 0.006
0.001 0.009 -0.001
0.012 0.009 -0.006

atensor 22 H
1.624 1.099 -1.450
1.099 -1.082 -0.541
-1.450 -0.541 -0.747
0.000 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.831 0.542 0.476
0.542 0.116 0.260
0.476 0.260 0.109
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.090 -0.015 0.006
-0.015 0.554 0.861
0.006 0.861 1.004
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.123 0.222 0.137
0.222 1.799 1.386
0.137 1.386 1.290
0.002 0.001 0.003
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.680 0.277 0.712
0.277 -0.684 2.061
0.712 2.061 2.734
0.005 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.013 -0.016

atensor 27 H
-0.826 -0.818 -1.066
-0.818 0.261 2.083
-1.066 2.083 1.178
0.006 0.001 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.487 0.624 -0.222
0.624 0.535 -0.102
-0.222 -0.102 -0.021
0.000 -0.005 0.001

0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
-0.073 0.282 -0.224
0.282 -2.559 -0.008
-0.224 -0.008 -1.694
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.234 1.821 0.401
1.821 0.461 0.637
0.401 0.637 0.728
0.039 -0.017 0.005
-0.033 0.009 -0.009
0.004 -0.011 0.067

atensor 31 H
2.163 1.272 0.591
1.272 -1.028 0.230
0.591 0.230 -1.341
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.007

atensor 32 H
0.981 1.224 2.263
1.224 -1.401 0.887
2.263 0.887 -0.158
-0.002 -0.006 -0.006
0.000 0.009 0.000
-0.013 -0.008 -0.001

atensor 33 H
-0.081 1.176 0.643
1.176 -0.340 0.555
0.643 0.555 -1.100
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.378 2.944 -0.452
2.944 0.407 -0.539
-0.452 -0.539 -3.994
0.010 -0.001 0.002
-0.009 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.192 -0.289 -0.111
-0.289 -0.720 0.037
-0.111 0.037 -0.723
-0.001 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.337 -0.372 -0.060
-0.372 0.152 0.035
-0.060 0.035 -0.219
-0.001 0.002 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.558 -0.586 -0.010
-0.586 0.537 0.030
-0.010 0.030 -0.794
-0.002 0.001 0.000
0.002 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.863 2.936 -0.258
2.936 27.658 -0.725
-0.258 -0.725 17.715
2.429 -0.364 0.113
-0.384 2.040 0.090
0.113 0.087 3.182

atensor 39 Cl
6.351 0.146 1.824
0.146 2.731 -4.905
1.824 -4.905 -6.066
0.474 0.039 0.038
0.036 0.256 -0.190
0.006 -0.267 0.347

atensor 40 Cl
4.614 1.091 -4.778
1.091 3.350 4.144
-4.778 4.144 -4.950
0.453 0.102 -0.075
0.082 0.286 0.180
-0.042 0.254 0.337

orbtensor 1 N
-476.767 51.958 48.516
51.958 -551.690 9.313
48.516 9.313 -96.157
338.521 -2.790 -2.014
-2.790 352.359 -0.683
-2.014 -0.683 322.569

orbtensor 2 C
-269.772 25.851 25.162
25.851 -298.646 4.626
25.162 4.626 -72.625
253.092 6.157 -5.665
6.157 252.127 -2.226
-5.665 -2.226 211.962

orbtensor 3 C
-222.771 -47.342 23.622
-47.342 -286.652 14.261
23.622 14.261 -57.225
252.337 3.889 -3.913
3.889 263.144 -1.894
-3.913 -1.894 223.832

orbtensor 4 C
-301.509 -22.132 32.894
-22.132 -231.418 9.044
32.894 9.044 -58.839
257.133 3.287 -5.268
3.287 253.321 -1.676
-5.268 -1.676 218.207

orbtensor 5 C
-287.597 2.684 30.137
2.684 -276.312 7.364

30.137	7.364	-59.009
269.078	0.621	-4.475
0.621	266.926	-1.201
-4.475	-1.201	235.409

orbtensor 6 C

-273.672	19.767	22.021
19.767	-298.093	4.353
22.021	4.353	-101.825
263.297	-4.674	-5.740
-4.674	261.723	-0.917
-5.740	-0.917	218.637

orbtensor 7 C

-295.829	12.610	30.563
12.610	-210.969	3.731
30.563	3.731	-61.195
257.851	-4.101	-5.085
-4.101	252.330	-0.679
-5.085	-0.679	218.275

orbtensor 8 C

-247.413	53.705	24.004
53.705	-272.020	0.832
24.004	0.832	-51.239
253.687	-5.371	-4.182
-5.371	256.250	-0.566
-4.182	-0.566	220.595

orbtensor 9 C

-236.953	-36.098	24.846
-36.098	-289.836	12.853
24.846	12.853	-58.877
253.125	-3.421	-4.280
-3.421	257.730	-0.897
-4.280	-0.897	219.825

orbtensor 10 C

-302.885	-14.652	28.573
-14.652	-250.073	7.595
28.573	7.595	-90.683
270.314	-0.813	-4.470
-0.813	265.280	-0.927
-4.470	-0.927	236.273

orbtensor 11 C

-220.827	33.177	0.122
33.177	-134.300	-6.951
0.122	-6.951	-210.845
250.310	-7.752	-1.266
-7.752	241.165	0.911
-1.266	0.911	238.629

orbtensor 12 C

-199.453	20.524	0.690
20.524	-106.842	24.199
0.690	24.199	-237.466
244.041	-2.650	-4.723
-2.650	236.024	-6.038
-4.723	-6.038	246.231

orbtensor 13 C

-228.891	-1.967	14.484
-1.967	-94.590	13.419
14.484	13.419	-220.823
247.773	3.495	-2.403
3.495	233.252	-4.285

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-2.403   -4.285   245.876

orbtensor 14 C
-202.472   12.149  -10.569
12.149  -111.077  -37.099
-10.569  -37.099  -230.176
246.527   -0.617   4.642
-0.617  236.930   7.016
4.642    7.016  242.838

orbtensor 15 C
-56.470    0.997    6.681
0.997  -48.559    2.873
6.681    2.873  -50.088
219.885   -0.322    2.564
-0.322  218.624   -4.258
2.564   -4.258  228.708

orbtensor 16 H
2.962   -0.721    0.101
-0.721    1.912    1.407
0.101    1.407    1.266
23.784    0.874   -0.628
0.874   29.299   -6.778
-0.628   -6.778   29.501

orbtensor 17 H
3.054    0.384   -1.960
0.384    3.379    2.362
-1.960    2.362    2.605
30.497   -0.478    0.421
-0.478   20.916   -2.417
0.421   -2.417   29.051

orbtensor 18 H
5.022    0.265   -0.055
0.265    3.316    2.180
-0.055    2.180   -1.453
21.577   -2.496   -0.447
-2.496   26.719    1.350
-0.447    1.350   30.585

orbtensor 19 C
-54.157   -0.468   -5.666
-0.468  -46.188    2.624
-5.666    2.624  -55.366
226.851    0.725   -6.853
0.725  218.951   -1.278
-6.853   -1.278  223.738

orbtensor 20 H
2.078   -0.616    1.178
-0.616    2.017    0.835
1.178    0.835    2.205
26.999    3.474   -4.146
3.474   28.744   -5.104
-4.146   -5.104   26.847

orbtensor 21 H
2.335   -1.557    2.987
-1.557    3.830    0.890
2.987    0.890    0.222
25.919    2.911   -3.047
2.911   25.013    3.340
-3.047    3.340   28.585

orbtensor 22 H

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-1.384	-0.860	1.455
-0.860	2.919	1.122
1.455	1.122	3.523
33.936	-2.111	-0.718
-2.111	22.554	-1.227
-0.718	-1.227	26.121

orbtensor 23 C

-51.425	-0.852	4.722
-0.852	-46.581	-3.159
4.722	-3.159	-57.708
230.007	1.472	5.098
1.472	219.126	1.194
5.098	1.194	220.408

orbtensor 24 C

-59.344	-0.148	-4.210
-0.148	-48.965	-2.956
-4.210	-2.956	-46.792
219.178	0.770	-0.147
0.770	219.255	4.888
-0.147	4.888	228.779

orbtensor 25 H

2.820	-1.078	-0.422
-1.078	1.729	-1.201
-0.422	-1.201	1.589
24.415	2.648	1.722
2.648	30.204	6.255
1.722	6.255	27.964

orbtensor 26 H

4.631	-0.390	-1.507
-0.390	2.994	-2.463
-1.507	-2.463	-0.741
22.440	-2.614	2.801
-2.614	26.589	-0.430
2.801	-0.430	29.854

orbtensor 27 H

3.998	-0.114	1.628
-0.114	3.047	-2.462
1.628	-2.462	1.997
30.190	0.192	-0.759
0.192	21.289	2.998
-0.759	2.998	28.982

orbtensor 28 H

-5.777	-6.386	0.619
-6.386	-16.718	1.316
0.619	1.316	-2.851
32.096	5.149	-1.294
5.149	41.605	-1.299
-1.294	-1.299	23.732

orbtensor 29 H

-18.504	-2.662	2.281
-2.662	-3.478	0.409
2.281	0.409	-1.965
41.673	2.199	-2.712
2.199	30.611	-0.607
-2.712	-0.607	21.760

orbtensor 30 C

-235.404	-7.251	-10.039
-7.251	-96.936	-20.510
-10.039	-20.510	-211.983

248.756	4.705	1.279
4.705	233.828	4.010
1.279	4.010	244.323

orbtensor 31 H

-1.762	-1.159	0.030
-1.159	2.788	-0.790
0.030	-0.790	4.033
33.813	-1.714	-1.205
-1.714	22.772	1.950
-1.205	1.950	26.028

orbtensor 32 H

0.752	-1.966	-2.990
-1.966	3.723	-0.620
-2.990	-0.620	1.907
27.559	2.209	3.202
2.209	24.528	-3.781
3.202	-3.781	27.428

orbtensor 33 H

1.519	-0.878	-0.931
-0.878	1.917	-0.601
-0.931	-0.601	2.862
28.951	4.889	3.212
4.889	29.357	3.775
3.212	3.775	24.283

orbtensor 34 H

-8.215	3.713	0.856
3.713	-14.390	-0.003
0.856	-0.003	-0.751
34.829	-1.316	-1.911
-1.316	36.463	-0.411
-1.911	-0.411	20.016

orbtensor 35 H

-18.329	0.609	2.094
0.609	-3.406	-0.031
2.094	-0.031	-2.308
42.213	-0.596	-2.651
-0.596	30.454	-0.230
-2.651	-0.230	21.988

orbtensor 36 H

-8.095	7.662	0.355
7.662	-13.776	-0.629
0.355	-0.629	-3.327
34.069	-6.703	-1.154
-6.703	38.535	0.341
-1.154	0.341	23.515

orbtensor 37 H

-5.360	-5.153	0.654
-5.153	-16.460	1.184
0.654	1.184	-1.827
31.636	1.659	-1.305
1.659	40.316	-0.852
-1.305	-0.852	22.234

orbtensor 38 Cr

-4995.561	438.282	-76.226
438.282	-3640.003	-119.878
-76.226	-119.878	-5452.191
1814.620	1.011	-0.424
1.011	1814.563	-0.233
-0.424	-0.233	1811.689


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orbtensor 39 Cl
-322.415  -20.258   15.031
-20.258  -460.519  164.382
15.031   164.382 -394.034
1141.122  -0.744   -2.553
-0.744  1145.107   5.235
-2.553   5.235  1146.575

```

```

orbtensor 40 Cl
-333.399  -62.189  -25.241
-62.189  -482.016 -147.288
-25.241  -147.288 -361.469
1142.777  -1.828   3.741
-1.828  1144.418  -4.803
3.741   -4.803  1145.611

```

```

gtensor (ppt)
-0.152   0.005   -0.001
0.005  -0.153   -0.001
-0.001  -0.001  -0.154
-3.907   3.399   -0.902
3.399  -2.988   -0.682
-0.902  -0.682   -9.807

```

```

zfstensor (cm-1)
-0.356084  -0.229342  -0.013134
-0.229342   0.748283   0.069207
-0.013134   0.069207  -0.392199

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.2393	-37.05500	4093.17163	-2.40277	4090.76885	4053.71385
2	C	3.6023	25.37933	-1892.46423	-1.48611	-1893.95034	-1868.57101
3	C	-0.6890	57.55500	361.96202	-0.52001	361.44201	418.99701
4	C	1.2713	45.63167	-667.88735	-0.38406	-668.27141	-622.63974
5	C	-1.1263	49.49833	591.71247	-0.12905	591.58342	641.08175
6	C	0.4670	23.35567	-245.33565	-0.50331	-245.83896	-222.48329
7	C	0.2437	53.48767	-128.00882	-0.01604	-128.02486	-74.53720
8	C	-0.3647	53.28667	191.57545	0.12720	191.70265	244.98931
9	C	-0.7590	48.33800	398.73610	0.35882	399.09492	447.43292
10	C	0.6087	42.74200	-319.75939	0.90336	-318.85603	-276.11403
11	C	-0.5263	54.71067	276.50606	0.63153	277.13760	331.84826
12	C	1.4093	60.84500	-740.38482	0.93137	-739.45345	-678.60845
13	C	1.1810	60.86567	-620.43127	-2.83790	-623.26917	-562.40350
14	C	1.4097	60.85667	-740.55994	1.63593	-738.92401	-678.06734
15	C	0.4917	170.70000	-258.29414	0.27971	-258.01442	-87.31442
16	H	1.0670	29.57467	-140.97847	0.13961	-140.83886	-111.26420
17	H	0.2030	29.83400	-26.82158	0.27616	-26.54542	3.28858
18	H	0.1217	28.58867	-16.07533	0.03793	-16.03740	12.55126
19	C	0.3563	171.27633	-187.19758	-0.87138	-188.06896	-16.79263
20	H	-0.5007	29.63000	66.15110	-0.32875	65.82234	95.45234
21	H	-0.1890	28.63467	24.97182	-0.54304	24.42878	53.06345
22	H	-0.0647	29.22300	8.54415	-0.72287	7.82128	37.04428
23	C	0.3560	171.27567	-187.02247	-0.80509	-187.82756	-16.55189
24	C	0.4937	170.70367	-259.34483	0.55237	-258.79246	-88.08879
25	H	1.0710	29.57367	-141.50698	0.25253	-141.25444	-111.68078
26	H	0.1220	28.58900	-16.11938	0.19102	-15.92835	12.66065
27	H	0.2043	29.83433	-26.99775	0.45085	-26.54690	3.28743
28	H	0.6680	24.02900	-88.26019	-0.29828	-88.55847	-64.52947
29	H	-1.4423	23.36567	190.56978	-0.40574	190.16404	213.52971
30	C	1.1793	60.86133	-619.55570	-2.61513	-622.17083	-561.30950
31	H	-0.0653	29.22400	8.63223	-0.70850	7.92373	37.14773
32	H	-0.1907	28.63233	25.19203	-0.50420	24.68783	53.32016
33	H	-0.5050	29.62967	66.72365	-0.28409	66.43955	96.06922

34	H	-1.6450	22.65067	217.34732	-0.58109	216.76623	239.41690
35	H	-0.4167	23.53733	55.05251	-0.04069	55.01182	78.54916
36	H	0.0897	23.64033	-11.84730	0.07801	-11.76930	11.87104
37	H	-0.2727	23.51300	36.02636	0.30600	36.33237	59.84537
38	Cr	23.9623	-2882.29433	55900.16835	-7.04451	55893.12384	53010.82951
39	Cl	1.3643	751.94533	-1837.68862	-7.72889	-1845.41751	-1093.47217
40	Cl	1.3633	751.97400	-1836.34167	-3.28086	-1839.62253	-1087.64853

=====
CrL1-STO-PBE-No-ZFS
Temperature: 295
Spin: 1.5

atensor 1 N
-1.263 0.234 -0.231
0.234 -2.139 -0.060
-0.231 -0.060 -2.942
-0.012 0.031 0.003
-0.004 0.030 0.000
0.005 -0.004 0.022

atensor 2 C
2.825 0.954 0.415
0.954 1.968 0.026
0.415 0.026 6.220
-0.049 0.013 0.006
0.012 0.007 -0.002
0.006 -0.002 0.003

atensor 3 C
0.254 0.160 -0.264
0.160 -0.402 -0.067
-0.264 -0.067 -1.699
0.001 -0.010 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C
0.189 0.071 0.526
0.071 -0.396 0.153
0.526 0.153 4.181
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.608 -0.091 -0.127
-0.091 -1.055 -0.008
-0.127 -0.008 -1.597
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.337 -0.514 -0.061
-0.514 -0.684 0.116
-0.061 0.116 0.734
0.006 0.001 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.116 -0.110 0.086
-0.110 -0.140 0.045
0.086 0.045 0.733
0.000 0.002 0.000

-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.140 -0.153 -0.065
-0.153 -0.215 0.004
-0.065 0.004 -0.671
-0.001 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.069 -0.247 0.126
-0.247 -0.926 0.059
0.126 0.059 -0.180
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.189 -0.947 -0.172
-0.946 0.937 0.077
-0.172 0.077 -0.371
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.005

atensor 11 C
0.067 -1.547 0.008
-1.547 -1.693 0.248
0.008 0.248 -0.296
0.059 0.019 0.002
-0.007 -0.016 0.004
0.003 0.001 0.083

atensor 12 C
0.179 -0.307 -0.007
-0.307 2.545 -2.304
-0.007 -2.304 1.312
0.061 0.000 0.000
-0.010 0.000 0.030
-0.009 0.028 0.043

atensor 13 C
1.853 1.577 -0.820
1.577 0.442 -1.053
-0.820 -1.053 1.110
0.039 -0.014 0.004
-0.029 0.010 0.021
0.005 0.019 0.066

atensor 14 C
0.250 0.288 0.246
0.288 2.857 2.199
0.246 2.199 0.929
0.062 -0.007 -0.004
-0.017 -0.003 -0.024
0.005 -0.024 0.046

atensor 15 C
-0.013 -0.219 0.287
-0.219 0.448 -0.790
0.287 -0.790 1.052
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.169 -0.140 0.192
-0.140 1.635 -1.416
0.192 -1.416 1.511
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.166 -1.221 1.521
-1.221 -0.022 -1.751
1.521 -1.751 0.749
0.003 0.004 -0.007
0.002 0.001 0.007
-0.008 0.012 -0.003

atensor 18 H
-1.728 -0.231 0.504
-0.231 -0.942 -1.795
0.504 -1.796 3.062
0.005 -0.003 -0.007
-0.003 0.009 0.004
0.000 0.013 -0.017

atensor 19 C
0.517 0.420 -0.617
0.420 0.052 -0.372
-0.617 -0.372 0.419
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.397 0.936 -0.871
0.936 -0.359 -0.861
-0.871 -0.861 -0.516
0.003 -0.003 0.001
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.195 0.809 -2.294
0.809 -1.497 -1.008
-2.294 -1.008 1.210
0.003 -0.004 0.006
0.001 0.009 -0.001
0.012 0.009 -0.007

atensor 22 H
1.623 1.093 -1.450
1.093 -1.080 -0.536
-1.450 -0.536 -0.745
-0.001 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.806 0.541 0.475
0.541 0.096 0.258
0.475 0.258 0.086
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.084 -0.014 0.006
-0.014 0.563 0.859

0.006 0.859 1.012
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.161 0.222 0.136
0.222 1.833 1.385
0.136 1.385 1.333
0.002 0.001 0.002
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.668 0.276 0.710
0.276 -0.675 2.051
0.710 2.051 2.738
0.006 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.014 -0.016

atensor 27 H
-0.843 -0.816 -1.064
-0.816 0.240 2.076
-1.064 2.076 1.165
0.006 0.002 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.416 0.635 -0.221
0.635 0.489 -0.103
-0.221 -0.103 -0.079
0.000 -0.006 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
0.012 0.278 -0.222
0.278 -2.452 -0.007
-0.222 -0.007 -1.593
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.176 1.839 0.402
1.839 0.554 0.634
0.402 0.634 0.669
0.039 -0.017 0.005
-0.033 0.008 -0.009
0.004 -0.011 0.068

atensor 31 H
2.162 1.265 0.591
1.265 -1.027 0.227
0.591 0.227 -1.338
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.008

atensor 32 H
1.008 1.217 2.259
1.217 -1.367 0.880
2.259 0.880 -0.127
-0.002 -0.006 -0.007
0.000 0.009 0.000

-0.013 -0.009 -0.001

atensor 33 H
0.002 1.174 0.646
1.174 -0.265 0.555
0.646 0.555 -1.020
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.217 2.939 -0.451
2.939 0.556 -0.537
-0.451 -0.537 -3.825
0.010 -0.002 0.002
-0.010 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.218 -0.289 -0.110
-0.289 -0.684 0.037
-0.110 0.037 -0.694
-0.002 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.311 -0.380 -0.059
-0.380 0.130 0.036
-0.059 0.036 -0.242
-0.001 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.524 -0.591 -0.011
-0.590 0.562 0.031
-0.011 0.031 -0.769
-0.002 0.002 0.000
0.003 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.919 2.924 -0.256
2.924 27.671 -0.722
-0.256 -0.722 17.783
2.468 -0.368 0.114
-0.389 2.062 0.091
0.114 0.089 3.227

atensor 39 Cl
6.405 0.149 1.807
0.149 2.872 -4.812
1.807 -4.812 -5.861
0.478 0.039 0.039
0.036 0.257 -0.194
0.007 -0.269 0.345

atensor 40 Cl
4.686 1.073 -4.725
1.073 3.479 4.058
-4.725 4.058 -4.751
0.456 0.103 -0.078
0.083 0.287 0.183
-0.044 0.255 0.336

orbtensor 1 N

-476.717	52.978	48.473
52.978	-550.776	9.150
48.473	9.150	-96.153
338.809	-2.897	-2.009
-2.897	352.351	-0.658
-2.009	-0.658	322.865

orbtensor 2 C

-269.174	25.637	25.237
25.637	-297.860	4.665
25.237	4.665	-71.524
252.707	6.254	-5.689
6.254	251.993	-2.253
-5.689	-2.253	211.419

orbtensor 3 C

-221.782	-47.753	23.591
-47.753	-286.635	14.336
23.591	14.336	-56.591
251.837	4.144	-3.908
4.144	263.164	-1.941
-3.908	-1.941	223.450

orbtensor 4 C

-300.826	-22.109	32.925
-22.109	-230.037	9.026
32.925	9.026	-57.921
256.860	3.386	-5.345
3.386	252.676	-1.695
-5.345	-1.695	217.378

orbtensor 5 C

-287.474	2.731	30.208
2.731	-276.128	7.375
30.208	7.375	-58.341
269.099	0.618	-4.477
0.618	266.808	-1.196
-4.477	-1.196	235.420

orbtensor 6 C

-272.935	19.878	22.096
19.878	-297.281	4.358
22.096	4.358	-100.487
262.956	-4.692	-5.776
-4.692	261.269	-0.921
-5.776	-0.921	218.012

orbtensor 7 C

-295.019	12.549	30.565
12.549	-209.717	3.723
30.565	3.723	-60.387
257.584	-4.214	-5.150
-4.214	251.624	-0.667
-5.150	-0.667	217.485

orbtensor 8 C

-246.524	54.065	23.970
54.065	-271.397	0.788
23.970	0.788	-50.511
253.237	-5.647	-4.158
-5.647	256.063	-0.536
-4.158	-0.536	220.248

orbtensor 9 C

-235.718	-36.206	24.820
-36.206	-289.186	12.879
24.820	12.879	-57.868

252.257	-3.416	-4.248
-3.416	257.500	-0.911
-4.248	-0.911	219.203

orbtensor 10 C

-302.334	-14.720	28.577
-14.720	-249.760	7.612
28.577	7.612	-90.131
269.898	-0.702	-4.435
-0.702	264.953	-0.933
-4.435	-0.933	236.153

orbtensor 11 C

-216.840	33.951	-0.010
33.951	-133.534	-6.969
-0.010	-6.969	-207.647
247.213	-8.374	-1.132
-8.374	240.702	0.930
-1.132	0.930	236.375

orbtensor 12 C

-197.072	20.279	0.960
20.279	-106.125	24.741
0.960	24.741	-235.160
242.584	-2.563	-5.096
-2.563	235.842	-6.480
-5.096	-6.480	244.419

orbtensor 13 C

-226.888	-2.622	14.205
-2.622	-93.565	13.901
14.205	13.901	-218.655
246.530	3.970	-1.974
3.970	232.821	-4.718
-1.974	-4.718	244.525

orbtensor 14 C

-200.225	11.772	-10.794
11.772	-110.423	-37.441
-10.794	-37.441	-227.677
245.230	-0.415	4.863
-0.415	236.799	7.298
4.863	7.298	240.819

orbtensor 15 C

-55.091	1.085	6.840
1.085	-47.047	3.027
6.840	3.027	-48.562
219.310	-0.423	2.591
-0.423	217.992	-4.410
2.591	-4.410	228.223

orbtensor 16 H

3.015	-0.715	0.117
-0.715	2.070	1.344
0.117	1.344	1.421
23.665	0.873	-0.654
0.873	29.131	-6.742
-0.654	-6.742	29.284

orbtensor 17 H

3.251	0.415	-1.957
0.415	3.393	2.410
-1.957	2.410	2.718
30.306	-0.501	0.409
-0.501	20.822	-2.445
0.409	-2.445	28.872


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orbtensor 18 H
5.063  0.272  -0.047
0.272  3.509  2.297
-0.047  2.297  -1.359
21.486  -2.517  -0.462
-2.517  26.516  1.295
-0.462  1.295  30.423

orbtensor 19 C
-52.749  -0.579  -5.730
-0.579  -44.560  2.738
-5.730  2.738  -53.879
226.398  0.802  -6.977
0.802  218.243  -1.354
-6.977  -1.354  223.109

orbtensor 20 H
2.170  -0.590  1.124
-0.590  2.183  0.781
1.124  0.781  2.339
26.844  3.468  -4.088
3.468  28.568  -5.083
-4.088  -5.083  26.661

orbtensor 21 H
2.383  -1.569  3.006
-1.569  4.029  1.005
3.006  1.005  0.335
25.815  2.924  -3.035
2.924  24.799  3.280
-3.035  3.280  28.425

orbtensor 22 H
-1.244  -0.961  1.479
-0.961  3.021  1.134
1.479  1.134  3.626
33.766  -2.051  -0.709
-2.051  22.395  -1.240
-0.709  -1.240  25.983

orbtensor 23 C
-49.979  -0.984  4.807
-0.984  -44.967  -3.251
4.807  -3.251  -56.246
229.602  1.572  5.157
1.572  218.427  1.250
5.157  1.250  219.721

orbtensor 24 C
-58.035  -0.110  -4.313
-0.110  -47.474  -3.119
-4.313  -3.119  -45.176
218.595  0.711  -0.146
0.711  218.645  5.070
-0.146  5.070  228.278

orbtensor 25 H
2.872  -1.055  -0.412
-1.055  1.897  -1.142
-0.412  -1.142  1.737
24.303  2.638  1.721
2.638  30.031  6.217
1.721  6.217  27.745

orbtensor 26 H
4.672  -0.414  -1.497

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-0.414	3.171	-2.584
-1.497	-2.584	-0.630
22.352	-2.619	2.796
-2.619	26.395	-0.370
2.796	-0.370	29.682

orbtensor 27 H

4.187	-0.097	1.604
-0.097	3.055	-2.509
1.604	-2.509	2.124
30.006	0.177	-0.745
0.177	21.199	3.024
-0.745	3.024	28.792

orbtensor 28 H

-5.802	-6.456	0.613
-6.456	-16.862	1.328
0.613	1.328	-2.939
32.111	5.145	-1.293
5.145	41.592	-1.297
-1.293	-1.297	23.751

orbtensor 29 H

-18.555	-2.657	2.289
-2.657	-3.445	0.408
2.289	0.408	-1.956
41.581	2.150	-2.707
2.150	30.595	-0.603
-2.707	-0.603	21.692

orbtensor 30 C

-233.241	-7.976	-9.703
-7.976	-95.958	-20.736
-9.703	-20.736	-209.928
247.284	5.237	0.840
5.237	233.442	4.253
0.840	4.253	243.154

orbtensor 31 H

-1.635	-1.262	0.008
-1.262	2.889	-0.775
0.008	-0.775	4.149
33.639	-1.652	-1.209
-1.652	22.613	1.948
-1.209	1.948	25.892

orbtensor 32 H

0.796	-2.009	-2.987
-2.009	3.907	-0.733
-2.987	-0.733	2.041
27.444	2.237	3.175
2.237	24.322	-3.723
3.175	-3.723	27.270

orbtensor 33 H

1.640	-0.835	-0.876
-0.835	2.089	-0.560
-0.876	-0.560	2.961
28.765	4.875	3.155
4.875	29.179	3.757
3.155	3.757	24.130

orbtensor 34 H

-8.285	3.628	0.872
3.628	-14.522	0.013
0.872	0.013	-0.726
34.865	-1.226	-1.925

-1.226 36.525 -0.426
-1.925 -0.426 19.973

orbtensor 35 H
-18.386 0.594 2.100
0.594 -3.383 -0.030
2.100 -0.030 -2.323
42.103 -0.562 -2.645
-0.562 30.441 -0.236
-2.645 -0.236 21.939

orbtensor 36 H
-8.100 7.726 0.341
7.726 -13.851 -0.638
0.341 -0.638 -3.419
34.019 -6.674 -1.147
-6.674 38.495 0.339
-1.147 0.339 23.525

orbtensor 37 H
-5.282 -5.242 0.636
-5.242 -16.483 1.193
0.636 1.193 -1.904
31.526 1.706 -1.292
1.706 40.212 -0.855
-1.292 -0.855 22.231

orbtensor 38 Cr
-5042.896 442.447 -78.204
442.447 -3681.490 -121.103
-78.204 -121.103 -5513.055
1814.989 0.961 -0.391
0.961 1814.311 -0.197
-0.391 -0.197 1812.293

orbtensor 39 Cl
-319.228 -19.524 15.304
-19.524 -458.010 162.180
15.304 162.180 -392.882
1141.478 -0.666 -2.532
-0.666 1145.000 4.821
-2.532 4.821 1146.531

orbtensor 40 Cl
-330.493 -61.001 -26.082
-61.001 -479.249 -145.433
-26.082 -145.433 -360.306
1143.092 -1.651 3.609
-1.651 1144.366 -4.421
3.609 -4.421 1145.551

gtensor (ppt)
-0.151 0.005 0.000
0.005 -0.152 -0.001
0.000 -0.001 -0.153
-4.178 3.424 -0.910
3.424 -3.206 -0.689
-0.910 -0.689 -10.132

averaging
2H Average:34
4H Average:29
9,10H Average:16,17,18,20,21,22
5H Average:35
8,11H Average:25,26,27,31,32,33
6H Average:36
3H Average:28

7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.1013	-36.54033	3840.41298	-2.15584	3838.25714	3801.71681
2	C	3.6580	25.85367	-1921.45073	0.97200	-1920.47873	-1894.62507
3	C	-0.6177	57.81433	324.44398	-0.72599	323.71798	381.53232
4	C	1.3187	46.04333	-692.66075	1.70045	-690.96030	-644.91697
5	C	-1.0847	49.79467	569.74674	-0.23514	569.51159	619.30626
6	C	0.4600	23.84467	-241.62584	0.56126	-241.06459	-217.21992
7	C	0.2350	53.85667	-123.43929	0.37746	-123.06183	-69.20516
8	C	-0.3427	53.70533	179.99374	-0.10203	179.89171	233.59705
9	C	-0.7267	48.72933	381.69880	0.48065	382.17945	430.90878
10	C	0.5837	42.92633	-306.58468	0.02530	-306.55937	-263.63304
11	C	-0.5987	55.42300	314.46378	1.25492	315.71870	371.14170
12	C	1.3800	61.49600	-724.87753	-0.20180	-725.07933	-663.58333
13	C	1.1733	61.58933	-616.32099	-1.12800	-617.44899	-555.85966
14	C	1.3803	61.50767	-725.05262	-0.20065	-725.25328	-663.74561
15	C	0.5000	171.60833	-262.63679	0.37579	-262.26100	-90.65266
16	H	1.1053	29.52867	-146.02372	0.02758	-145.99615	-116.46748
17	H	0.1873	29.78733	-24.74829	0.26987	-24.47843	5.30891
18	H	0.1297	28.54600	-17.13004	0.40687	-16.72317	11.82283
19	C	0.3333	172.18733	-175.09119	-0.32197	-175.41316	-3.22582
20	H	-0.4220	29.58833	55.74971	-0.21572	55.53399	85.12233
21	H	-0.1590	28.59533	21.00522	-0.03705	20.96817	49.56351
22	H	-0.0640	29.18233	8.45493	-0.30613	8.14880	37.33113
23	C	0.3333	172.18600	-175.09119	-0.32187	-175.41306	-3.22706
24	C	0.5013	171.61100	-263.33715	0.37581	-262.96134	-91.35034
25	H	1.1093	29.52833	-146.55216	0.02778	-146.52438	-116.99605
26	H	0.1307	28.54733	-17.26215	0.40713	-16.85502	11.69231
27	H	0.1873	29.78767	-24.74829	0.27033	-24.47796	5.30971
28	H	0.6097	23.95033	-80.54204	-0.19493	-80.73696	-56.78663
29	H	-1.3447	23.30400	177.64165	-0.05981	177.58184	200.88584
30	C	1.1713	61.58433	-615.27045	-1.12569	-616.39613	-554.81180
31	H	-0.0640	29.18233	8.45493	-0.30601	8.14892	37.33126
32	H	-0.1600	28.59333	21.13733	-0.03685	21.10048	49.69382
33	H	-0.4257	29.58800	56.23411	-0.21549	56.01861	85.60661
34	H	-1.4853	22.61000	196.22488	-0.82605	195.39884	218.00884
35	H	-0.3867	23.46367	51.08188	0.00653	51.08841	74.55208
36	H	0.0660	23.55633	-8.71915	0.01423	-8.70492	14.85141
37	H	-0.2447	23.43333	32.32250	0.00362	32.32612	55.75945
38	Cr	24.0433	-2931.94933	56081.60798	16.42733	56098.03531	53166.08598
39	Cl	1.4987	754.29633	-2018.35825	-10.85488	-2029.21312	-1274.91679
40	Cl	1.4977	754.32033	-2017.01148	-10.84413	-2027.85561	-1273.53528

=====
CrL1-STO-PBE-Neese

Temperature: 295

Spin: 1.5

atensor 1 N

-1.263 0.234 -0.231
0.234 -2.139 -0.060
-0.231 -0.060 -2.942
-0.012 0.031 0.003
-0.004 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.825 0.954 0.415
0.954 1.968 0.026
0.415 0.026 6.220
-0.049 0.013 0.006
0.012 0.007 -0.002

0.006 -0.002 0.003

atensor 3 C
0.254 0.160 -0.264
0.160 -0.402 -0.067
-0.264 -0.067 -1.699
0.001 -0.010 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C
0.189 0.071 0.526
0.071 -0.396 0.153
0.526 0.153 4.181
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.608 -0.091 -0.127
-0.091 -1.055 -0.008
-0.127 -0.008 -1.597
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.337 -0.514 -0.061
-0.514 -0.684 0.116
-0.061 0.116 0.734
0.006 0.001 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.116 -0.110 0.086
-0.110 -0.140 0.045
0.086 0.045 0.733
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.140 -0.153 -0.065
-0.153 -0.215 0.004
-0.065 0.004 -0.671
-0.001 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.069 -0.247 0.126
-0.247 -0.926 0.059
0.126 0.059 -0.180
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.189 -0.947 -0.172
-0.946 0.937 0.077
-0.172 0.077 -0.371
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.005

atensor 11 C

0.067 -1.547 0.008
-1.547 -1.693 0.248
0.008 0.248 -0.296
0.059 0.019 0.002
-0.007 -0.016 0.004
0.003 0.001 0.083

atensor 12 C
0.179 -0.307 -0.007
-0.307 2.545 -2.304
-0.007 -2.304 1.312
0.061 0.000 0.000
-0.010 0.000 0.030
-0.009 0.028 0.043

atensor 13 C
1.853 1.577 -0.820
1.577 0.442 -1.053
-0.820 -1.053 1.110
0.039 -0.014 0.004
-0.029 0.010 0.021
0.005 0.019 0.066

atensor 14 C
0.250 0.288 0.246
0.288 2.857 2.199
0.246 2.199 0.929
0.062 -0.007 -0.004
-0.017 -0.003 -0.024
0.005 -0.024 0.046

atensor 15 C
-0.013 -0.219 0.287
-0.219 0.448 -0.790
0.287 -0.790 1.052
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.169 -0.140 0.192
-0.140 1.635 -1.416
0.192 -1.416 1.511
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.166 -1.221 1.521
-1.221 -0.022 -1.751
1.521 -1.751 0.749
0.003 0.004 -0.007
0.002 0.001 0.007
-0.008 0.012 -0.003

atensor 18 H
-1.728 -0.231 0.504
-0.231 -0.942 -1.795
0.504 -1.796 3.062
0.005 -0.003 -0.007
-0.003 0.009 0.004
0.000 0.013 -0.017

atensor 19 C
0.517 0.420 -0.617
0.420 0.052 -0.372
-0.617 -0.372 0.419

0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.397 0.936 -0.871
0.936 -0.359 -0.861
-0.871 -0.861 -0.516
0.003 -0.003 0.001
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.195 0.809 -2.294
0.809 -1.497 -1.008
-2.294 -1.008 1.210
0.003 -0.004 0.006
0.001 0.009 -0.001
0.012 0.009 -0.007

atensor 22 H
1.623 1.093 -1.450
1.093 -1.080 -0.536
-1.450 -0.536 -0.745
-0.001 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.806 0.541 0.475
0.541 0.096 0.258
0.475 0.258 0.086
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.084 -0.014 0.006
-0.014 0.563 0.859
0.006 0.859 1.012
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.161 0.222 0.136
0.222 1.833 1.385
0.136 1.385 1.333
0.002 0.001 0.002
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.668 0.276 0.710
0.276 -0.675 2.051
0.710 2.051 2.738
0.006 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.014 -0.016

atensor 27 H
-0.843 -0.816 -1.064
-0.816 0.240 2.076
-1.064 2.076 1.165
0.006 0.002 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.416 0.635 -0.221
0.635 0.489 -0.103
-0.221 -0.103 -0.079
0.000 -0.006 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
0.012 0.278 -0.222
0.278 -2.452 -0.007
-0.222 -0.007 -1.593
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.176 1.839 0.402
1.839 0.554 0.634
0.402 0.634 0.669
0.039 -0.017 0.005
-0.033 0.008 -0.009
0.004 -0.011 0.068

atensor 31 H
2.162 1.265 0.591
1.265 -1.027 0.227
0.591 0.227 -1.338
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.008

atensor 32 H
1.008 1.217 2.259
1.217 -1.367 0.880
2.259 0.880 -0.127
-0.002 -0.006 -0.007
0.000 0.009 0.000
-0.013 -0.009 -0.001

atensor 33 H
0.002 1.174 0.646
1.174 -0.265 0.555
0.646 0.555 -1.020
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.217 2.939 -0.451
2.939 0.556 -0.537
-0.451 -0.537 -3.825
0.010 -0.002 0.002
-0.010 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.218 -0.289 -0.110
-0.289 -0.684 0.037
-0.110 0.037 -0.694
-0.002 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.311 -0.380 -0.059

-0.380 0.130 0.036
-0.059 0.036 -0.242
-0.001 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.524 -0.591 -0.011
-0.590 0.562 0.031
-0.011 0.031 -0.769
-0.002 0.002 0.000
0.003 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.919 2.924 -0.256
2.924 27.671 -0.722
-0.256 -0.722 17.783
2.468 -0.368 0.114
-0.389 2.062 0.091
0.114 0.089 3.227

atensor 39 Cl
6.405 0.149 1.807
0.149 2.872 -4.812
1.807 -4.812 -5.861
0.478 0.039 0.039
0.036 0.257 -0.194
0.007 -0.269 0.345

atensor 40 Cl
4.686 1.073 -4.725
1.073 3.479 4.058
-4.725 4.058 -4.751
0.456 0.103 -0.078
0.083 0.287 0.183
-0.044 0.255 0.336

orbtensor 1 N
-476.717 52.978 48.473
52.978 -550.776 9.150
48.473 9.150 -96.153
338.809 -2.897 -2.009
-2.897 352.351 -0.658
-2.009 -0.658 322.865

orbtensor 2 C
-269.174 25.637 25.237
25.637 -297.860 4.665
25.237 4.665 -71.524
252.707 6.254 -5.689
6.254 251.993 -2.253
-5.689 -2.253 211.419

orbtensor 3 C
-221.782 -47.753 23.591
-47.753 -286.635 14.336
23.591 14.336 -56.591
251.837 4.144 -3.908
4.144 263.164 -1.941
-3.908 -1.941 223.450

orbtensor 4 C
-300.826 -22.109 32.925
-22.109 -230.037 9.026
32.925 9.026 -57.921
256.860 3.386 -5.345

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3.386 252.676 -1.695
-5.345 -1.695 217.378

orbtensor 5 C
-287.474 2.731 30.208
2.731 -276.128 7.375
30.208 7.375 -58.341
269.099 0.618 -4.477
0.618 266.808 -1.196
-4.477 -1.196 235.420

orbtensor 6 C
-272.935 19.878 22.096
19.878 -297.281 4.358
22.096 4.358 -100.487
262.956 -4.692 -5.776
-4.692 261.269 -0.921
-5.776 -0.921 218.012

orbtensor 7 C
-295.019 12.549 30.565
12.549 -209.717 3.723
30.565 3.723 -60.387
257.584 -4.214 -5.150
-4.214 251.624 -0.667
-5.150 -0.667 217.485

orbtensor 8 C
-246.524 54.065 23.970
54.065 -271.397 0.788
23.970 0.788 -50.511
253.237 -5.647 -4.158
-5.647 256.063 -0.536
-4.158 -0.536 220.248

orbtensor 9 C
-235.718 -36.206 24.820
-36.206 -289.186 12.879
24.820 12.879 -57.868
252.257 -3.416 -4.248
-3.416 257.500 -0.911
-4.248 -0.911 219.203

orbtensor 10 C
-302.334 -14.720 28.577
-14.720 -249.760 7.612
28.577 7.612 -90.131
269.898 -0.702 -4.435
-0.702 264.953 -0.933
-4.435 -0.933 236.153

orbtensor 11 C
-216.840 33.951 -0.010
33.951 -133.534 -6.969
-0.010 -6.969 -207.647
247.213 -8.374 -1.132
-8.374 240.702 0.930
-1.132 0.930 236.375

orbtensor 12 C
-197.072 20.279 0.960
20.279 -106.125 24.741
0.960 24.741 -235.160
242.584 -2.563 -5.096
-2.563 235.842 -6.480
-5.096 -6.480 244.419

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orbtensor 13 C
-226.888 -2.622 14.205
-2.622 -93.565 13.901
14.205 13.901 -218.655
246.530 3.970 -1.974
3.970 232.821 -4.718
-1.974 -4.718 244.525

orbtensor 14 C
-200.225 11.772 -10.794
11.772 -110.423 -37.441
-10.794 -37.441 -227.677
245.230 -0.415 4.863
-0.415 236.799 7.298
4.863 7.298 240.819

orbtensor 15 C
-55.091 1.085 6.840
1.085 -47.047 3.027
6.840 3.027 -48.562
219.310 -0.423 2.591
-0.423 217.992 -4.410
2.591 -4.410 228.223

orbtensor 16 H
3.015 -0.715 0.117
-0.715 2.070 1.344
0.117 1.344 1.421
23.665 0.873 -0.654
0.873 29.131 -6.742
-0.654 -6.742 29.284

orbtensor 17 H
3.251 0.415 -1.957
0.415 3.393 2.410
-1.957 2.410 2.718
30.306 -0.501 0.409
-0.501 20.822 -2.445
0.409 -2.445 28.872

orbtensor 18 H
5.063 0.272 -0.047
0.272 3.509 2.297
-0.047 2.297 -1.359
21.486 -2.517 -0.462
-2.517 26.516 1.295
-0.462 1.295 30.423

orbtensor 19 C
-52.749 -0.579 -5.730
-0.579 -44.560 2.738
-5.730 2.738 -53.879
226.398 0.802 -6.977
0.802 218.243 -1.354
-6.977 -1.354 223.109

orbtensor 20 H
2.170 -0.590 1.124
-0.590 2.183 0.781
1.124 0.781 2.339
26.844 3.468 -4.088
3.468 28.568 -5.083
-4.088 -5.083 26.661

orbtensor 21 H
2.383 -1.569 3.006
-1.569 4.029 1.005

3.006	1.005	0.335
25.815	2.924	-3.035
2.924	24.799	3.280
-3.035	3.280	28.425

orbtensor 22 H

-1.244	-0.961	1.479
-0.961	3.021	1.134
1.479	1.134	3.626
33.766	-2.051	-0.709
-2.051	22.395	-1.240
-0.709	-1.240	25.983

orbtensor 23 C

-49.979	-0.984	4.807
-0.984	-44.967	-3.251
4.807	-3.251	-56.246
229.602	1.572	5.157
1.572	218.427	1.250
5.157	1.250	219.721

orbtensor 24 C

-58.035	-0.110	-4.313
-0.110	-47.474	-3.119
-4.313	-3.119	-45.176
218.595	0.711	-0.146
0.711	218.645	5.070
-0.146	5.070	228.278

orbtensor 25 H

2.872	-1.055	-0.412
-1.055	1.897	-1.142
-0.412	-1.142	1.737
24.303	2.638	1.721
2.638	30.031	6.217
1.721	6.217	27.745

orbtensor 26 H

4.672	-0.414	-1.497
-0.414	3.171	-2.584
-1.497	-2.584	-0.630
22.352	-2.619	2.796
-2.619	26.395	-0.370
2.796	-0.370	29.682

orbtensor 27 H

4.187	-0.097	1.604
-0.097	3.055	-2.509
1.604	-2.509	2.124
30.006	0.177	-0.745
0.177	21.199	3.024
-0.745	3.024	28.792

orbtensor 28 H

-5.802	-6.456	0.613
-6.456	-16.862	1.328
0.613	1.328	-2.939
32.111	5.145	-1.293
5.145	41.592	-1.297
-1.293	-1.297	23.751

orbtensor 29 H

-18.555	-2.657	2.289
-2.657	-3.445	0.408
2.289	0.408	-1.956
41.581	2.150	-2.707
2.150	30.595	-0.603

```

-2.707   -0.603   21.692

orbtensor 30 C
-233.241  -7.976  -9.703
-7.976  -95.958  -20.736
-9.703  -20.736  -209.928
247.284   5.237   0.840
5.237  233.442   4.253
0.840   4.253  243.154

orbtensor 31 H
-1.635  -1.262   0.008
-1.262   2.889  -0.775
0.008  -0.775   4.149
33.639  -1.652  -1.209
-1.652  22.613   1.948
-1.209   1.948  25.892

orbtensor 32 H
0.796  -2.009  -2.987
-2.009   3.907  -0.733
-2.987  -0.733   2.041
27.444   2.237   3.175
2.237  24.322  -3.723
3.175  -3.723  27.270

orbtensor 33 H
1.640  -0.835  -0.876
-0.835   2.089  -0.560
-0.876  -0.560   2.961
28.765   4.875   3.155
4.875  29.179   3.757
3.155   3.757  24.130

orbtensor 34 H
-8.285   3.628   0.872
3.628  -14.522   0.013
0.872   0.013  -0.726
34.865  -1.226  -1.925
-1.226  36.525  -0.426
-1.925  -0.426  19.973

orbtensor 35 H
-18.386   0.594   2.100
0.594  -3.383  -0.030
2.100  -0.030  -2.323
42.103  -0.562  -2.645
-0.562  30.441  -0.236
-2.645  -0.236  21.939

orbtensor 36 H
-8.100   7.726   0.341
7.726  -13.851  -0.638
0.341  -0.638  -3.419
34.019  -6.674  -1.147
-6.674  38.495   0.339
-1.147   0.339  23.525

orbtensor 37 H
-5.282  -5.242   0.636
-5.242  -16.483   1.193
0.636   1.193  -1.904
31.526   1.706  -1.292
1.706  40.212  -0.855
-1.292  -0.855  22.231

orbtensor 38 Cr

```

```

-5042.896  442.447  -78.204
442.447 -3681.490  -121.103
-78.204  -121.103 -5513.055
1814.989    0.961  -0.391
0.961  1814.311  -0.197
-0.391   -0.197  1812.293

```

```

orbtensor 39 C1
-319.228  -19.524   15.304
-19.524 -458.010  162.180
15.304  162.180 -392.882
1141.478   -0.666   -2.532
-0.666  1145.000   4.821
-2.532    4.821  1146.531

```

```

orbtensor 40 C1
-330.493  -61.001  -26.082
-61.001 -479.249 -145.433
-26.082 -145.433 -360.306
1143.092  -1.651   3.609
-1.651  1144.366  -4.421
3.609   -4.421  1145.551

```

```

gtensor (ppt)
-0.151    0.005    0.000
0.005   -0.152   -0.001
0.000   -0.001   -0.153
-4.178    3.424   -0.910
3.424   -3.206   -0.689
-0.910   -0.689  -10.132

```

```

zfstensor (cm-1)
-0.438630  -0.175757    0.025038
-0.175757    0.639815    0.051714
0.025038    0.051714   -0.201185

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.1013	-36.54033	3840.41113	-3.24435	3837.16679	3800.62645
2	C	3.6580	25.85367	-1921.44981	-0.57123	-1922.02104	-1896.16737
3	C	-0.6177	57.81433	324.44382	-0.83605	323.60777	381.42211
4	C	1.3187	46.04333	-692.66042	0.52207	-692.13835	-646.09502
5	C	-1.0847	49.79467	569.74646	-0.29502	569.45145	619.24611
6	C	0.4600	23.84467	-241.62573	-0.44475	-242.07047	-218.22581
7	C	0.2350	53.85667	-123.43923	0.13105	-123.30818	-69.45151
8	C	-0.3427	53.70533	179.99366	0.00779	180.00145	233.70678
9	C	-0.7267	48.72933	381.69861	0.50124	382.19986	430.92919
10	C	0.5837	42.92633	-306.58453	0.50918	-306.07535	-263.14902
11	C	-0.5987	55.42300	314.46363	0.70860	315.17223	370.59523
12	C	1.3800	61.49600	-724.87718	0.94025	-723.93693	-662.44093
13	C	1.1733	61.58933	-616.32070	-2.62220	-618.94289	-557.35356
14	C	1.3803	61.50767	-725.05227	1.45750	-723.59478	-662.08711
15	C	0.5000	171.60833	-262.63666	0.46442	-262.17224	-90.56391
16	H	1.1053	29.52867	-146.02365	0.17584	-145.84782	-116.31915
17	H	0.1873	29.78733	-24.74828	0.32930	-24.41898	5.36836
18	H	0.1297	28.54600	-17.13004	0.27189	-16.85815	11.68785
19	C	0.3333	172.18733	-175.09111	-0.82474	-175.91585	-3.72852
20	H	-0.4220	29.58833	55.74968	-0.32126	55.42842	85.01676
21	H	-0.1590	28.59533	21.00521	-0.44858	20.55663	49.15197
22	H	-0.0640	29.18233	8.45493	-0.75583	7.69910	36.88143
23	C	0.3333	172.18600	-175.09111	-0.77805	-175.86916	-3.68316
24	C	0.5013	171.61100	-263.33702	0.66382	-262.67320	-91.06220
25	H	1.1093	29.52833	-146.55209	0.25866	-146.29342	-116.76509
26	H	0.1307	28.54733	-17.26214	0.38348	-16.87867	11.66867
27	H	0.1873	29.78767	-24.74828	0.45769	-24.29059	5.49708

28	H	0.6097	23.95033	-80.54200	-0.33234	-80.87434	-56.92400
29	H	-1.3447	23.30400	177.64156	-0.40751	177.23405	200.53805
30	C	1.1713	61.58433	-615.27015	-2.45884	-617.72899	-556.14466
31	H	-0.0640	29.18233	8.45493	-0.74617	7.70875	36.89109
32	H	-0.1600	28.59333	21.13732	-0.42173	20.71559	49.30892
33	H	-0.4257	29.58800	56.23408	-0.28905	55.94503	85.53303
34	H	-1.4853	22.61000	196.22479	-0.68856	195.53623	218.14623
35	H	-0.3867	23.46367	51.08186	-0.06856	51.01330	74.47697
36	H	0.0660	23.55633	-8.71914	0.04699	-8.67215	14.88418
37	H	-0.2447	23.43333	32.32249	0.24662	32.56910	56.00244
38	Cr	24.0433	-2931.94933	56081.58100	-3.62679	56077.95421	53146.00488
39	Cl	1.4987	754.29633	-2018.35728	-11.91461	-2030.27188	-1275.97555
40	Cl	1.4977	754.32033	-2017.01051	-8.68753	-2025.69803	-1271.37770

=====
 CrL1-STO-PBE-ORCA

Temperature: 295

Spin: 1.5

atensor 1 N

-1.263 0.234 -0.231
 0.234 -2.139 -0.060
 -0.231 -0.060 -2.942
 -0.012 0.031 0.003
 -0.004 0.030 0.000
 0.005 -0.004 0.022

atensor 2 C

2.825 0.954 0.415
 0.954 1.968 0.026
 0.415 0.026 6.220
 -0.049 0.013 0.006
 0.012 0.007 -0.002
 0.006 -0.002 0.003

atensor 3 C

0.254 0.160 -0.264
 0.160 -0.402 -0.067
 -0.264 -0.067 -1.699
 0.001 -0.010 0.000
 0.002 -0.008 0.000
 0.000 0.002 0.001

atensor 4 C

0.189 0.071 0.526
 0.071 -0.396 0.153
 0.526 0.153 4.181
 -0.009 0.004 0.001
 0.001 -0.009 0.000
 0.001 0.000 0.000

atensor 5 C

-0.608 -0.091 -0.127
 -0.091 -1.055 -0.008
 -0.127 -0.008 -1.597
 -0.001 -0.003 0.000
 0.000 0.005 0.000
 0.000 0.000 0.002

atensor 6 C

1.337 -0.514 -0.061
 -0.514 -0.684 0.116
 -0.061 0.116 0.734
 0.006 0.001 -0.001
 -0.019 -0.014 0.003
 0.000 0.000 0.001

atensor 7 C
0.116 -0.110 0.086
-0.110 -0.140 0.045
0.086 0.045 0.733
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.140 -0.153 -0.065
-0.153 -0.215 0.004
-0.065 0.004 -0.671
-0.001 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.069 -0.247 0.126
-0.247 -0.926 0.059
0.126 0.059 -0.180
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.189 -0.947 -0.172
-0.946 0.937 0.077
-0.172 0.077 -0.371
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.005

atensor 11 C
0.067 -1.547 0.008
-1.547 -1.693 0.248
0.008 0.248 -0.296
0.059 0.019 0.002
-0.007 -0.016 0.004
0.003 0.001 0.083

atensor 12 C
0.179 -0.307 -0.007
-0.307 2.545 -2.304
-0.007 -2.304 1.312
0.061 0.000 0.000
-0.010 0.000 0.030
-0.009 0.028 0.043

atensor 13 C
1.853 1.577 -0.820
1.577 0.442 -1.053
-0.820 -1.053 1.110
0.039 -0.014 0.004
-0.029 0.010 0.021
0.005 0.019 0.066

atensor 14 C
0.250 0.288 0.246
0.288 2.857 2.199
0.246 2.199 0.929
0.062 -0.007 -0.004
-0.017 -0.003 -0.024
0.005 -0.024 0.046

atensor 15 C
-0.013 -0.219 0.287

-0.219 0.448 -0.790
0.287 -0.790 1.052
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.169 -0.140 0.192
-0.140 1.635 -1.416
0.192 -1.416 1.511
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.166 -1.221 1.521
-1.221 -0.022 -1.751
1.521 -1.751 0.749
0.003 0.004 -0.007
0.002 0.001 0.007
-0.008 0.012 -0.003

atensor 18 H
-1.728 -0.231 0.504
-0.231 -0.942 -1.795
0.504 -1.796 3.062
0.005 -0.003 -0.007
-0.003 0.009 0.004
0.000 0.013 -0.017

atensor 19 C
0.517 0.420 -0.617
0.420 0.052 -0.372
-0.617 -0.372 0.419
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.397 0.936 -0.871
0.936 -0.359 -0.861
-0.871 -0.861 -0.516
0.003 -0.003 0.001
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.195 0.809 -2.294
0.809 -1.497 -1.008
-2.294 -1.008 1.210
0.003 -0.004 0.006
0.001 0.009 -0.001
0.012 0.009 -0.007

atensor 22 H
1.623 1.093 -1.450
1.093 -1.080 -0.536
-1.450 -0.536 -0.745
-0.001 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.806 0.541 0.475
0.541 0.096 0.258
0.475 0.258 0.086
0.002 -0.004 -0.003

-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.084 -0.014 0.006
-0.014 0.563 0.859
0.006 0.859 1.012
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.161 0.222 0.136
0.222 1.833 1.385
0.136 1.385 1.333
0.002 0.001 0.002
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.668 0.276 0.710
0.276 -0.675 2.051
0.710 2.051 2.738
0.006 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.014 -0.016

atensor 27 H
-0.843 -0.816 -1.064
-0.816 0.240 2.076
-1.064 2.076 1.165
0.006 0.002 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.416 0.635 -0.221
0.635 0.489 -0.103
-0.221 -0.103 -0.079
0.000 -0.006 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
0.012 0.278 -0.222
0.278 -2.452 -0.007
-0.222 -0.007 -1.593
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.176 1.839 0.402
1.839 0.554 0.634
0.402 0.634 0.669
0.039 -0.017 0.005
-0.033 0.008 -0.009
0.004 -0.011 0.068

atensor 31 H
2.162 1.265 0.591
1.265 -1.027 0.227
0.591 0.227 -1.338
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.008

atensor 32 H
1.008 1.217 2.259
1.217 -1.367 0.880
2.259 0.880 -0.127
-0.002 -0.006 -0.007
0.000 0.009 0.000
-0.013 -0.009 -0.001

atensor 33 H
0.002 1.174 0.646
1.174 -0.265 0.555
0.646 0.555 -1.020
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.217 2.939 -0.451
2.939 0.556 -0.537
-0.451 -0.537 -3.825
0.010 -0.002 0.002
-0.010 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.218 -0.289 -0.110
-0.289 -0.684 0.037
-0.110 0.037 -0.694
-0.002 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.311 -0.380 -0.059
-0.380 0.130 0.036
-0.059 0.036 -0.242
-0.001 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.524 -0.591 -0.011
-0.590 0.562 0.031
-0.011 0.031 -0.769
-0.002 0.002 0.000
0.003 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.919 2.924 -0.256
2.924 27.671 -0.722
-0.256 -0.722 17.783
2.468 -0.368 0.114
-0.389 2.062 0.091
0.114 0.089 3.227

atensor 39 Cl
6.405 0.149 1.807
0.149 2.872 -4.812
1.807 -4.812 -5.861
0.478 0.039 0.039
0.036 0.257 -0.194
0.007 -0.269 0.345

atensor 40 Cl
4.686 1.073 -4.725
1.073 3.479 4.058

-4.725 4.058 -4.751
0.456 0.103 -0.078
0.083 0.287 0.183
-0.044 0.255 0.336

orbtensor 1 N
-476.717 52.978 48.473
52.978 -550.776 9.150
48.473 9.150 -96.153
338.809 -2.897 -2.009
-2.897 352.351 -0.658
-2.009 -0.658 322.865

orbtensor 2 C
-269.174 25.637 25.237
25.637 -297.860 4.665
25.237 4.665 -71.524
252.707 6.254 -5.689
6.254 251.993 -2.253
-5.689 -2.253 211.419

orbtensor 3 C
-221.782 -47.753 23.591
-47.753 -286.635 14.336
23.591 14.336 -56.591
251.837 4.144 -3.908
4.144 263.164 -1.941
-3.908 -1.941 223.450

orbtensor 4 C
-300.826 -22.109 32.925
-22.109 -230.037 9.026
32.925 9.026 -57.921
256.860 3.386 -5.345
3.386 252.676 -1.695
-5.345 -1.695 217.378

orbtensor 5 C
-287.474 2.731 30.208
2.731 -276.128 7.375
30.208 7.375 -58.341
269.099 0.618 -4.477
0.618 266.808 -1.196
-4.477 -1.196 235.420

orbtensor 6 C
-272.935 19.878 22.096
19.878 -297.281 4.358
22.096 4.358 -100.487
262.956 -4.692 -5.776
-4.692 261.269 -0.921
-5.776 -0.921 218.012

orbtensor 7 C
-295.019 12.549 30.565
12.549 -209.717 3.723
30.565 3.723 -60.387
257.584 -4.214 -5.150
-4.214 251.624 -0.667
-5.150 -0.667 217.485

orbtensor 8 C
-246.524 54.065 23.970
54.065 -271.397 0.788
23.970 0.788 -50.511
253.237 -5.647 -4.158
-5.647 256.063 -0.536

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-4.158   -0.536   220.248

orbtensor 9 C
-235.718  -36.206   24.820
-36.206  -289.186   12.879
24.820   12.879  -57.868
252.257  -3.416   -4.248
-3.416   257.500  -0.911
-4.248   -0.911  219.203

orbtensor 10 C
-302.334  -14.720   28.577
-14.720  -249.760   7.612
28.577    7.612  -90.131
269.898  -0.702  -4.435
-0.702   264.953  -0.933
-4.435   -0.933  236.153

orbtensor 11 C
-216.840   33.951  -0.010
33.951  -133.534  -6.969
-0.010   -6.969 -207.647
247.213   -8.374  -1.132
-8.374   240.702   0.930
-1.132    0.930  236.375

orbtensor 12 C
-197.072   20.279   0.960
20.279  -106.125   24.741
0.960   24.741 -235.160
242.584   -2.563  -5.096
-2.563   235.842  -6.480
-5.096   -6.480  244.419

orbtensor 13 C
-226.888   -2.622   14.205
-2.622  -93.565   13.901
14.205   13.901 -218.655
246.530    3.970  -1.974
3.970   232.821  -4.718
-1.974   -4.718  244.525

orbtensor 14 C
-200.225   11.772  -10.794
11.772 -110.423  -37.441
-10.794  -37.441 -227.677
245.230   -0.415   4.863
-0.415   236.799   7.298
4.863    7.298  240.819

orbtensor 15 C
-55.091    1.085   6.840
1.085  -47.047   3.027
6.840    3.027  -48.562
219.310   -0.423   2.591
-0.423   217.992  -4.410
2.591   -4.410  228.223

orbtensor 16 H
3.015   -0.715   0.117
-0.715    2.070   1.344
0.117    1.344   1.421
23.665    0.873  -0.654
0.873   29.131  -6.742
-0.654   -6.742  29.284

orbtensor 17 H

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3.251	0.415	-1.957
0.415	3.393	2.410
-1.957	2.410	2.718
30.306	-0.501	0.409
-0.501	20.822	-2.445
0.409	-2.445	28.872

orbtensor 18 H

5.063	0.272	-0.047
0.272	3.509	2.297
-0.047	2.297	-1.359
21.486	-2.517	-0.462
-2.517	26.516	1.295
-0.462	1.295	30.423

orbtensor 19 C

-52.749	-0.579	-5.730
-0.579	-44.560	2.738
-5.730	2.738	-53.879
226.398	0.802	-6.977
0.802	218.243	-1.354
-6.977	-1.354	223.109

orbtensor 20 H

2.170	-0.590	1.124
-0.590	2.183	0.781
1.124	0.781	2.339
26.844	3.468	-4.088
3.468	28.568	-5.083
-4.088	-5.083	26.661

orbtensor 21 H

2.383	-1.569	3.006
-1.569	4.029	1.005
3.006	1.005	0.335
25.815	2.924	-3.035
2.924	24.799	3.280
-3.035	3.280	28.425

orbtensor 22 H

-1.244	-0.961	1.479
-0.961	3.021	1.134
1.479	1.134	3.626
33.766	-2.051	-0.709
-2.051	22.395	-1.240
-0.709	-1.240	25.983

orbtensor 23 C

-49.979	-0.984	4.807
-0.984	-44.967	-3.251
4.807	-3.251	-56.246
229.602	1.572	5.157
1.572	218.427	1.250
5.157	1.250	219.721

orbtensor 24 C

-58.035	-0.110	-4.313
-0.110	-47.474	-3.119
-4.313	-3.119	-45.176
218.595	0.711	-0.146
0.711	218.645	5.070
-0.146	5.070	228.278

orbtensor 25 H

2.872	-1.055	-0.412
-1.055	1.897	-1.142
-0.412	-1.142	1.737

24.303	2.638	1.721
2.638	30.031	6.217
1.721	6.217	27.745

orbtensor 26 H

4.672	-0.414	-1.497
-0.414	3.171	-2.584
-1.497	-2.584	-0.630
22.352	-2.619	2.796
-2.619	26.395	-0.370
2.796	-0.370	29.682

orbtensor 27 H

4.187	-0.097	1.604
-0.097	3.055	-2.509
1.604	-2.509	2.124
30.006	0.177	-0.745
0.177	21.199	3.024
-0.745	3.024	28.792

orbtensor 28 H

-5.802	-6.456	0.613
-6.456	-16.862	1.328
0.613	1.328	-2.939
32.111	5.145	-1.293
5.145	41.592	-1.297
-1.293	-1.297	23.751

orbtensor 29 H

-18.555	-2.657	2.289
-2.657	-3.445	0.408
2.289	0.408	-1.956
41.581	2.150	-2.707
2.150	30.595	-0.603
-2.707	-0.603	21.692

orbtensor 30 C

-233.241	-7.976	-9.703
-7.976	-95.958	-20.736
-9.703	-20.736	-209.928
247.284	5.237	0.840
5.237	233.442	4.253
0.840	4.253	243.154

orbtensor 31 H

-1.635	-1.262	0.008
-1.262	2.889	-0.775
0.008	-0.775	4.149
33.639	-1.652	-1.209
-1.652	22.613	1.948
-1.209	1.948	25.892

orbtensor 32 H

0.796	-2.009	-2.987
-2.009	3.907	-0.733
-2.987	-0.733	2.041
27.444	2.237	3.175
2.237	24.322	-3.723
3.175	-3.723	27.270

orbtensor 33 H

1.640	-0.835	-0.876
-0.835	2.089	-0.560
-0.876	-0.560	2.961
28.765	4.875	3.155
4.875	29.179	3.757
3.155	3.757	24.130

```

orbtensor 34 H
-8.285    3.628    0.872
 3.628  -14.522    0.013
 0.872    0.013   -0.726
34.865  -1.226   -1.925
-1.226   36.525   -0.426
-1.925   -0.426   19.973

orbtensor 35 H
-18.386    0.594    2.100
 0.594   -3.383   -0.030
 2.100   -0.030   -2.323
42.103   -0.562   -2.645
-0.562   30.441   -0.236
-2.645   -0.236   21.939

orbtensor 36 H
-8.100    7.726    0.341
 7.726  -13.851   -0.638
 0.341   -0.638   -3.419
34.019   -6.674   -1.147
-6.674   38.495    0.339
-1.147    0.339   23.525

orbtensor 37 H
-5.282   -5.242    0.636
-5.242  -16.483    1.193
 0.636    1.193   -1.904
31.526    1.706   -1.292
 1.706   40.212   -0.855
-1.292   -0.855   22.231

orbtensor 38 Cr
-5042.896  442.447  -78.204
442.447 -3681.490 -121.103
-78.204 -121.103 -5513.055
1814.989    0.961   -0.391
 0.961 1814.311   -0.197
-0.391   -0.197 1812.293

orbtensor 39 Cl
-319.228  -19.524   15.304
-19.524 -458.010  162.180
15.304  162.180 -392.882
1141.478   -0.666   -2.532
-0.666 1145.000    4.821
-2.532    4.821 1146.531

orbtensor 40 Cl
-330.493  -61.001  -26.082
-61.001 -479.249 -145.433
-26.082 -145.433 -360.306
1143.092   -1.651    3.609
-1.651 1144.366   -4.421
 3.609   -4.421 1145.551

gtensor (ppt)
-0.151    0.005    0.000
 0.005   -0.152   -0.001
 0.000   -0.001   -0.153
-4.178    3.424   -0.910
 3.424   -3.206   -0.689
-0.910   -0.689  -10.132

zfstensor (cm-1)
-1.007854    0.221707    0.026536

```


0.221707 0.270629 -0.063929
 0.026536 -0.063929 -0.747226

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.1013	-36.54033	3840.39884	-2.57164	3837.82720	3801.28687
2	C	3.6580	25.85367	-1921.44366	-0.07823	-1921.52188	-1895.66822
3	C	-0.6177	57.81433	324.44278	-0.67802	323.76476	381.57909
4	C	1.3187	46.04333	-692.65820	0.26266	-692.39554	-646.35220
5	C	-1.0847	49.79467	569.74464	-0.37289	569.37175	619.16642
6	C	0.4600	23.84467	-241.62495	-1.12373	-242.74868	-218.90401
7	C	0.2350	53.85667	-123.43884	-0.03322	-123.47206	-69.61539
8	C	-0.3427	53.70533	179.99308	-0.09615	179.89694	233.60227
9	C	-0.7267	48.72933	381.69739	0.25787	381.95526	430.68460
10	C	0.5837	42.92633	-306.58355	-0.22480	-306.80835	-263.88201
11	C	-0.5987	55.42300	314.46262	-0.81109	313.65153	369.07453
12	C	1.3800	61.49600	-724.87486	1.45846	-723.41640	-661.92040
13	C	1.1733	61.58933	-616.31872	-1.27256	-617.59128	-556.00195
14	C	1.3803	61.50767	-725.04995	1.46058	-723.58937	-662.08171
15	C	0.5000	171.60833	-262.63582	0.47421	-262.16161	-90.55327
16	H	1.1053	29.52867	-146.02319	0.26043	-145.76276	-116.23409
17	H	0.1873	29.78733	-24.74820	0.17842	-24.56978	5.21755
18	H	0.1297	28.54600	-17.12998	0.29280	-16.83718	11.70882
19	C	0.3333	172.18733	-175.09055	-0.45773	-175.54828	-3.36094
20	H	-0.4220	29.58833	55.74950	-0.07888	55.67062	85.25896
21	H	-0.1590	28.59533	21.00514	-0.28694	20.71821	49.31354
22	H	-0.0640	29.18233	8.45490	-0.55973	7.89517	37.07751
23	C	0.3333	172.18600	-175.09055	-0.45667	-175.54722	-3.36122
24	C	0.5013	171.61100	-263.33618	0.47444	-262.86174	-91.25074
25	H	1.1093	29.52833	-146.55162	0.26062	-146.29099	-116.76266
26	H	0.1307	28.54733	-17.26209	0.29268	-16.96941	11.57792
27	H	0.1873	29.78767	-24.74820	0.17777	-24.57043	5.21724
28	H	0.6097	23.95033	-80.54174	-0.20829	-80.75003	-56.79970
29	H	-1.3447	23.30400	177.64099	-0.40876	177.23223	200.53623
30	C	1.1713	61.58433	-615.26818	-1.27338	-616.54156	-554.95723
31	H	-0.0640	29.18233	8.45490	-0.55946	7.89544	37.07777
32	H	-0.1600	28.59333	21.13725	-0.28638	20.85088	49.44421
33	H	-0.4257	29.58800	56.23390	-0.07873	56.15517	85.74317
34	H	-1.4853	22.61000	196.22416	0.02908	196.25324	218.86324
35	H	-0.3867	23.46367	51.08169	-0.14627	50.93543	74.39909
36	H	0.0660	23.55633	-8.71912	-0.03049	-8.74961	14.80673
37	H	-0.2447	23.43333	32.32238	0.16342	32.48580	55.91914
38	Cr	24.0433	-2931.94933	56081.40144	-18.23366	56063.16778	53131.21844
39	Cl	1.4987	754.29633	-2018.35081	-8.04527	-2026.39608	-1272.09975
40	Cl	1.4977	754.32033	-2017.00405	-8.04912	-2025.05317	-1270.73284

=====
 CrL1-STO-PBE-Pederson

Temperature: 295

Spin: 1.5

atensor 1 N

-1.263 0.234 -0.231
 0.234 -2.139 -0.060
 -0.231 -0.060 -2.942
 -0.012 0.031 0.003
 -0.004 0.030 0.000
 0.005 -0.004 0.022

atensor 2 C

2.825 0.954 0.415
 0.954 1.968 0.026
 0.415 0.026 6.220
 -0.049 0.013 0.006

0.012 0.007 -0.002
0.006 -0.002 0.003

atensor 3 C
0.254 0.160 -0.264
0.160 -0.402 -0.067
-0.264 -0.067 -1.699
0.001 -0.010 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C
0.189 0.071 0.526
0.071 -0.396 0.153
0.526 0.153 4.181
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C
-0.608 -0.091 -0.127
-0.091 -1.055 -0.008
-0.127 -0.008 -1.597
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C
1.337 -0.514 -0.061
-0.514 -0.684 0.116
-0.061 0.116 0.734
0.006 0.001 -0.001
-0.019 -0.014 0.003
0.000 0.000 0.001

atensor 7 C
0.116 -0.110 0.086
-0.110 -0.140 0.045
0.086 0.045 0.733
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.140 -0.153 -0.065
-0.153 -0.215 0.004
-0.065 0.004 -0.671
-0.001 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.069 -0.247 0.126
-0.247 -0.926 0.059
0.126 0.059 -0.180
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.189 -0.947 -0.172
-0.946 0.937 0.077
-0.172 0.077 -0.371
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.005

atensor 11 C
0.067 -1.547 0.008
-1.547 -1.693 0.248
0.008 0.248 -0.296
0.059 0.019 0.002
-0.007 -0.016 0.004
0.003 0.001 0.083

atensor 12 C
0.179 -0.307 -0.007
-0.307 2.545 -2.304
-0.007 -2.304 1.312
0.061 0.000 0.000
-0.010 0.000 0.030
-0.009 0.028 0.043

atensor 13 C
1.853 1.577 -0.820
1.577 0.442 -1.053
-0.820 -1.053 1.110
0.039 -0.014 0.004
-0.029 0.010 0.021
0.005 0.019 0.066

atensor 14 C
0.250 0.288 0.246
0.288 2.857 2.199
0.246 2.199 0.929
0.062 -0.007 -0.004
-0.017 -0.003 -0.024
0.005 -0.024 0.046

atensor 15 C
-0.013 -0.219 0.287
-0.219 0.448 -0.790
0.287 -0.790 1.052
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.169 -0.140 0.192
-0.140 1.635 -1.416
0.192 -1.416 1.511
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.166 -1.221 1.521
-1.221 -0.022 -1.751
1.521 -1.751 0.749
0.003 0.004 -0.007
0.002 0.001 0.007
-0.008 0.012 -0.003

atensor 18 H
-1.728 -0.231 0.504
-0.231 -0.942 -1.795
0.504 -1.796 3.062
0.005 -0.003 -0.007
-0.003 0.009 0.004
0.000 0.013 -0.017

atensor 19 C
0.517 0.420 -0.617
0.420 0.052 -0.372

-0.617 -0.372 0.419
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.397 0.936 -0.871
0.936 -0.359 -0.861
-0.871 -0.861 -0.516
0.003 -0.003 0.001
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.195 0.809 -2.294
0.809 -1.497 -1.008
-2.294 -1.008 1.210
0.003 -0.004 0.006
0.001 0.009 -0.001
0.012 0.009 -0.007

atensor 22 H
1.623 1.093 -1.450
1.093 -1.080 -0.536
-1.450 -0.536 -0.745
-0.001 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.806 0.541 0.475
0.541 0.096 0.258
0.475 0.258 0.086
0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.084 -0.014 0.006
-0.014 0.563 0.859
0.006 0.859 1.012
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.161 0.222 0.136
0.222 1.833 1.385
0.136 1.385 1.333
0.002 0.001 0.002
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.668 0.276 0.710
0.276 -0.675 2.051
0.710 2.051 2.738
0.006 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.014 -0.016

atensor 27 H
-0.843 -0.816 -1.064
-0.816 0.240 2.076
-1.064 2.076 1.165
0.006 0.002 0.004
0.000 -0.001 -0.007

0.005 -0.013 -0.005

atensor 28 H
1.416 0.635 -0.221
0.635 0.489 -0.103
-0.221 -0.103 -0.079
0.000 -0.006 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
0.012 0.278 -0.222
0.278 -2.452 -0.007
-0.222 -0.007 -1.593
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.176 1.839 0.402
1.839 0.554 0.634
0.402 0.634 0.669
0.039 -0.017 0.005
-0.033 0.008 -0.009
0.004 -0.011 0.068

atensor 31 H
2.162 1.265 0.591
1.265 -1.027 0.227
0.591 0.227 -1.338
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.008

atensor 32 H
1.008 1.217 2.259
1.217 -1.367 0.880
2.259 0.880 -0.127
-0.002 -0.006 -0.007
0.000 0.009 0.000
-0.013 -0.009 -0.001

atensor 33 H
0.002 1.174 0.646
1.174 -0.265 0.555
0.646 0.555 -1.020
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.217 2.939 -0.451
2.939 0.556 -0.537
-0.451 -0.537 -3.825
0.010 -0.002 0.002
-0.010 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.218 -0.289 -0.110
-0.289 -0.684 0.037
-0.110 0.037 -0.694
-0.002 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H

0.311 -0.380 -0.059
-0.380 0.130 0.036
-0.059 0.036 -0.242
-0.001 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.524 -0.591 -0.011
-0.590 0.562 0.031
-0.011 0.031 -0.769
-0.002 0.002 0.000
0.003 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.919 2.924 -0.256
2.924 27.671 -0.722
-0.256 -0.722 17.783
2.468 -0.368 0.114
-0.389 2.062 0.091
0.114 0.089 3.227

atensor 39 Cl
6.405 0.149 1.807
0.149 2.872 -4.812
1.807 -4.812 -5.861
0.478 0.039 0.039
0.036 0.257 -0.194
0.007 -0.269 0.345

atensor 40 Cl
4.686 1.073 -4.725
1.073 3.479 4.058
-4.725 4.058 -4.751
0.456 0.103 -0.078
0.083 0.287 0.183
-0.044 0.255 0.336

orbtensor 1 N
-476.717 52.978 48.473
52.978 -550.776 9.150
48.473 9.150 -96.153
338.809 -2.897 -2.009
-2.897 352.351 -0.658
-2.009 -0.658 322.865

orbtensor 2 C
-269.174 25.637 25.237
25.637 -297.860 4.665
25.237 4.665 -71.524
252.707 6.254 -5.689
6.254 251.993 -2.253
-5.689 -2.253 211.419

orbtensor 3 C
-221.782 -47.753 23.591
-47.753 -286.635 14.336
23.591 14.336 -56.591
251.837 4.144 -3.908
4.144 263.164 -1.941
-3.908 -1.941 223.450

orbtensor 4 C
-300.826 -22.109 32.925
-22.109 -230.037 9.026
32.925 9.026 -57.921

256.860	3.386	-5.345
3.386	252.676	-1.695
-5.345	-1.695	217.378

orbtensor 5 C

-287.474	2.731	30.208
2.731	-276.128	7.375
30.208	7.375	-58.341
269.099	0.618	-4.477
0.618	266.808	-1.196
-4.477	-1.196	235.420

orbtensor 6 C

-272.935	19.878	22.096
19.878	-297.281	4.358
22.096	4.358	-100.487
262.956	-4.692	-5.776
-4.692	261.269	-0.921
-5.776	-0.921	218.012

orbtensor 7 C

-295.019	12.549	30.565
12.549	-209.717	3.723
30.565	3.723	-60.387
257.584	-4.214	-5.150
-4.214	251.624	-0.667
-5.150	-0.667	217.485

orbtensor 8 C

-246.524	54.065	23.970
54.065	-271.397	0.788
23.970	0.788	-50.511
253.237	-5.647	-4.158
-5.647	256.063	-0.536
-4.158	-0.536	220.248

orbtensor 9 C

-235.718	-36.206	24.820
-36.206	-289.186	12.879
24.820	12.879	-57.868
252.257	-3.416	-4.248
-3.416	257.500	-0.911
-4.248	-0.911	219.203

orbtensor 10 C

-302.334	-14.720	28.577
-14.720	-249.760	7.612
28.577	7.612	-90.131
269.898	-0.702	-4.435
-0.702	264.953	-0.933
-4.435	-0.933	236.153

orbtensor 11 C

-216.840	33.951	-0.010
33.951	-133.534	-6.969
-0.010	-6.969	-207.647
247.213	-8.374	-1.132
-8.374	240.702	0.930
-1.132	0.930	236.375

orbtensor 12 C

-197.072	20.279	0.960
20.279	-106.125	24.741
0.960	24.741	-235.160
242.584	-2.563	-5.096
-2.563	235.842	-6.480
-5.096	-6.480	244.419

orbtensor 13 C
-226.888 -2.622 14.205
-2.622 -93.565 13.901
14.205 13.901 -218.655
246.530 3.970 -1.974
3.970 232.821 -4.718
-1.974 -4.718 244.525

orbtensor 14 C
-200.225 11.772 -10.794
11.772 -110.423 -37.441
-10.794 -37.441 -227.677
245.230 -0.415 4.863
-0.415 236.799 7.298
4.863 7.298 240.819

orbtensor 15 C
-55.091 1.085 6.840
1.085 -47.047 3.027
6.840 3.027 -48.562
219.310 -0.423 2.591
-0.423 217.992 -4.410
2.591 -4.410 228.223

orbtensor 16 H
3.015 -0.715 0.117
-0.715 2.070 1.344
0.117 1.344 1.421
23.665 0.873 -0.654
0.873 29.131 -6.742
-0.654 -6.742 29.284

orbtensor 17 H
3.251 0.415 -1.957
0.415 3.393 2.410
-1.957 2.410 2.718
30.306 -0.501 0.409
-0.501 20.822 -2.445
0.409 -2.445 28.872

orbtensor 18 H
5.063 0.272 -0.047
0.272 3.509 2.297
-0.047 2.297 -1.359
21.486 -2.517 -0.462
-2.517 26.516 1.295
-0.462 1.295 30.423

orbtensor 19 C
-52.749 -0.579 -5.730
-0.579 -44.560 2.738
-5.730 2.738 -53.879
226.398 0.802 -6.977
0.802 218.243 -1.354
-6.977 -1.354 223.109

orbtensor 20 H
2.170 -0.590 1.124
-0.590 2.183 0.781
1.124 0.781 2.339
26.844 3.468 -4.088
3.468 28.568 -5.083
-4.088 -5.083 26.661

orbtensor 21 H
2.383 -1.569 3.006

-1.569	4.029	1.005
3.006	1.005	0.335
25.815	2.924	-3.035
2.924	24.799	3.280
-3.035	3.280	28.425

orbtensor 22 H

-1.244	-0.961	1.479
-0.961	3.021	1.134
1.479	1.134	3.626
33.766	-2.051	-0.709
-2.051	22.395	-1.240
-0.709	-1.240	25.983

orbtensor 23 C

-49.979	-0.984	4.807
-0.984	-44.967	-3.251
4.807	-3.251	-56.246
229.602	1.572	5.157
1.572	218.427	1.250
5.157	1.250	219.721

orbtensor 24 C

-58.035	-0.110	-4.313
-0.110	-47.474	-3.119
-4.313	-3.119	-45.176
218.595	0.711	-0.146
0.711	218.645	5.070
-0.146	5.070	228.278

orbtensor 25 H

2.872	-1.055	-0.412
-1.055	1.897	-1.142
-0.412	-1.142	1.737
24.303	2.638	1.721
2.638	30.031	6.217
1.721	6.217	27.745

orbtensor 26 H

4.672	-0.414	-1.497
-0.414	3.171	-2.584
-1.497	-2.584	-0.630
22.352	-2.619	2.796
-2.619	26.395	-0.370
2.796	-0.370	29.682

orbtensor 27 H

4.187	-0.097	1.604
-0.097	3.055	-2.509
1.604	-2.509	2.124
30.006	0.177	-0.745
0.177	21.199	3.024
-0.745	3.024	28.792

orbtensor 28 H

-5.802	-6.456	0.613
-6.456	-16.862	1.328
0.613	1.328	-2.939
32.111	5.145	-1.293
5.145	41.592	-1.297
-1.293	-1.297	23.751

orbtensor 29 H

-18.555	-2.657	2.289
-2.657	-3.445	0.408
2.289	0.408	-1.956
41.581	2.150	-2.707

2.150	30.595	-0.603
-2.707	-0.603	21.692

orbtensor 30 C

-233.241	-7.976	-9.703
-7.976	-95.958	-20.736
-9.703	-20.736	-209.928
247.284	5.237	0.840
5.237	233.442	4.253
0.840	4.253	243.154

orbtensor 31 H

-1.635	-1.262	0.008
-1.262	2.889	-0.775
0.008	-0.775	4.149
33.639	-1.652	-1.209
-1.652	22.613	1.948
-1.209	1.948	25.892

orbtensor 32 H

0.796	-2.009	-2.987
-2.009	3.907	-0.733
-2.987	-0.733	2.041
27.444	2.237	3.175
2.237	24.322	-3.723
3.175	-3.723	27.270

orbtensor 33 H

1.640	-0.835	-0.876
-0.835	2.089	-0.560
-0.876	-0.560	2.961
28.765	4.875	3.155
4.875	29.179	3.757
3.155	3.757	24.130

orbtensor 34 H

-8.285	3.628	0.872
3.628	-14.522	0.013
0.872	0.013	-0.726
34.865	-1.226	-1.925
-1.226	36.525	-0.426
-1.925	-0.426	19.973

orbtensor 35 H

-18.386	0.594	2.100
0.594	-3.383	-0.030
2.100	-0.030	-2.323
42.103	-0.562	-2.645
-0.562	30.441	-0.236
-2.645	-0.236	21.939

orbtensor 36 H

-8.100	7.726	0.341
7.726	-13.851	-0.638
0.341	-0.638	-3.419
34.019	-6.674	-1.147
-6.674	38.495	0.339
-1.147	0.339	23.525

orbtensor 37 H

-5.282	-5.242	0.636
-5.242	-16.483	1.193
0.636	1.193	-1.904
31.526	1.706	-1.292
1.706	40.212	-0.855
-1.292	-0.855	22.231

```

orbtensor 38 Cr
-5042.896  442.447  -78.204
442.447 -3681.490  -121.103
-78.204  -121.103 -5513.055
1814.989   0.961   -0.391
0.961 1814.311   -0.197
-0.391  -0.197 1812.293

```

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orbtensor 39 Cl
-319.228  -19.524  15.304
-19.524  -458.010  162.180
15.304  162.180  -392.882
1141.478   -0.666   -2.532
-0.666 1145.000   4.821
-2.532   4.821 1146.531

```

```

orbtensor 40 Cl
-330.493  -61.001  -26.082
-61.001  -479.249  -145.433
-26.082  -145.433  -360.306
1143.092   -1.651   3.609
-1.651 1144.366   -4.421
3.609  -4.421 1145.551

```

```

gtensor (ppt)
-0.151   0.005   0.000
0.005  -0.152  -0.001
0.000  -0.001  -0.153
-4.178   3.424  -0.910
3.424  -3.206  -0.689
-0.910  -0.689 -10.132

```

```

zfstensor (cm-1)
-0.241509  -0.157458  -0.009299
-0.157458   0.510002   0.047345
-0.009299   0.047345  -0.268494

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.1013	-36.54033	3840.40939	-2.38224	3838.02715	3801.48682
2	C	3.6580	25.85367	-1921.44894	-0.69415	-1922.14309	-1896.28942
3	C	-0.6177	57.81433	324.44367	-0.59034	323.85333	381.66767
4	C	1.3187	46.04333	-692.66011	0.29104	-692.36907	-646.32573
5	C	-1.0847	49.79467	569.74620	-0.16413	569.58207	619.37674
6	C	0.4600	23.84467	-241.62562	-0.15034	-241.77595	-217.93129
7	C	0.2350	53.85667	-123.43917	0.11279	-123.32638	-69.46972
8	C	-0.3427	53.70533	179.99358	0.05273	180.04631	233.75164
9	C	-0.7267	48.72933	381.69844	0.40069	382.09913	430.82847
10	C	0.5837	42.92633	-306.58439	0.62565	-305.95874	-263.03240
11	C	-0.5987	55.42300	314.46349	0.91333	315.37682	370.79982
12	C	1.3800	61.49600	-724.87685	0.56949	-724.30736	-662.81136
13	C	1.1733	61.58933	-616.32042	-2.25943	-618.57985	-556.99052
14	C	1.3803	61.50767	-725.05195	1.05083	-724.00111	-662.49345
15	C	0.5000	171.60833	-262.63654	0.31198	-262.32457	-90.71623
16	H	1.1053	29.52867	-146.02359	0.10280	-145.92079	-116.39213
17	H	0.1873	29.78733	-24.74827	0.27493	-24.47334	5.31399
18	H	0.1297	28.54600	-17.13003	0.15692	-16.97311	11.57289
19	C	0.3333	172.18733	-175.09103	-0.69486	-175.78589	-3.59855
20	H	-0.4220	29.58833	55.74966	-0.29448	55.45517	85.04351
21	H	-0.1590	28.59533	21.00520	-0.37965	20.62556	49.22089
22	H	-0.0640	29.18233	8.45492	-0.58916	7.86576	37.04809
23	C	0.3333	172.18600	-175.09103	-0.65077	-175.74180	-3.55580
24	C	0.5013	171.61100	-263.33691	0.49737	-262.83954	-91.22854
25	H	1.1093	29.52833	-146.55202	0.17985	-146.37217	-116.84383
26	H	0.1307	28.54733	-17.26214	0.26089	-17.00124	11.54609

27	H	0.1873	29.78767	-24.74827	0.39407	-24.35420	5.43347
28	H	0.6097	23.95033	-80.54196	-0.26596	-80.80792	-56.85759
29	H	-1.3447	23.30400	177.64148	-0.29201	177.34947	200.65347
30	C	1.1713	61.58433	-615.26987	-2.10622	-617.37609	-555.79176
31	H	-0.0640	29.18233	8.45492	-0.57981	7.87511	37.05745
32	H	-0.1600	28.59333	21.13731	-0.35384	20.78347	49.37680
33	H	-0.4257	29.58800	56.23405	-0.26421	55.96985	85.55785
34	H	-1.4853	22.61000	196.22470	-0.66586	195.55884	218.16884
35	H	-0.3867	23.46367	51.08183	-0.02398	51.05785	74.52152
36	H	0.0660	23.55633	-8.71914	0.05986	-8.65928	14.89705
37	H	-0.2447	23.43333	32.32247	0.20937	32.53184	55.96517
38	Cr	24.0433	-2931.94933	56081.55556	0.65716	56082.21272	53150.26339
39	Cl	1.4987	754.29633	-2018.35636	-8.67170	-2027.02806	-1272.73172
40	Cl	1.4977	754.32033	-2017.00959	-5.68160	-2022.69119	-1268.37086

=====
CrL1-STO-PBE-Van-Wullen

Temperature: 295

Spin: 1.5

atensor 1 N

-1.263 0.234 -0.231
0.234 -2.139 -0.060
-0.231 -0.060 -2.942
-0.012 0.031 0.003
-0.004 0.030 0.000
0.005 -0.004 0.022

atensor 2 C

2.825 0.954 0.415
0.954 1.968 0.026
0.415 0.026 6.220
-0.049 0.013 0.006
0.012 0.007 -0.002
0.006 -0.002 0.003

atensor 3 C

0.254 0.160 -0.264
0.160 -0.402 -0.067
-0.264 -0.067 -1.699
0.001 -0.010 0.000
0.002 -0.008 0.000
0.000 0.002 0.001

atensor 4 C

0.189 0.071 0.526
0.071 -0.396 0.153
0.526 0.153 4.181
-0.009 0.004 0.001
0.001 -0.009 0.000
0.001 0.000 0.000

atensor 5 C

-0.608 -0.091 -0.127
-0.091 -1.055 -0.008
-0.127 -0.008 -1.597
-0.001 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.002

atensor 6 C

1.337 -0.514 -0.061
-0.514 -0.684 0.116
-0.061 0.116 0.734
0.006 0.001 -0.001
-0.019 -0.014 0.003

0.000 0.000 0.001

atensor 7 C
0.116 -0.110 0.086
-0.110 -0.140 0.045
0.086 0.045 0.733
0.000 0.002 0.000
-0.001 -0.004 0.000
0.000 0.000 0.000

atensor 8 C
-0.140 -0.153 -0.065
-0.153 -0.215 0.004
-0.065 0.004 -0.671
-0.001 0.005 0.000
0.001 -0.001 0.000
0.000 -0.001 0.000

atensor 9 C
-1.069 -0.247 0.126
-0.247 -0.926 0.059
0.126 0.059 -0.180
-0.009 -0.010 0.001
0.002 0.004 0.000
0.001 0.001 0.000

atensor 10 C
1.189 -0.947 -0.172
-0.946 0.937 0.077
-0.172 0.077 -0.371
0.000 -0.005 0.001
0.007 -0.009 0.000
0.000 0.001 0.005

atensor 11 C
0.067 -1.547 0.008
-1.547 -1.693 0.248
0.008 0.248 -0.296
0.059 0.019 0.002
-0.007 -0.016 0.004
0.003 0.001 0.083

atensor 12 C
0.179 -0.307 -0.007
-0.307 2.545 -2.304
-0.007 -2.304 1.312
0.061 0.000 0.000
-0.010 0.000 0.030
-0.009 0.028 0.043

atensor 13 C
1.853 1.577 -0.820
1.577 0.442 -1.053
-0.820 -1.053 1.110
0.039 -0.014 0.004
-0.029 0.010 0.021
0.005 0.019 0.066

atensor 14 C
0.250 0.288 0.246
0.288 2.857 2.199
0.246 2.199 0.929
0.062 -0.007 -0.004
-0.017 -0.003 -0.024
0.005 -0.024 0.046

atensor 15 C

-0.013 -0.219 0.287
-0.219 0.448 -0.790
0.287 -0.790 1.052
0.011 0.000 -0.004
-0.002 0.001 0.004
-0.003 0.006 0.001

atensor 16 H
0.169 -0.140 0.192
-0.140 1.635 -1.416
0.192 -1.416 1.511
0.002 0.002 -0.003
0.000 0.000 0.004
0.001 0.007 -0.001

atensor 17 H
-0.166 -1.221 1.521
-1.221 -0.022 -1.751
1.521 -1.751 0.749
0.003 0.004 -0.007
0.002 0.001 0.007
-0.008 0.012 -0.003

atensor 18 H
-1.728 -0.231 0.504
-0.231 -0.942 -1.795
0.504 -1.796 3.062
0.005 -0.003 -0.007
-0.003 0.009 0.004
0.000 0.013 -0.017

atensor 19 C
0.517 0.420 -0.617
0.420 0.052 -0.372
-0.617 -0.372 0.419
0.005 -0.004 0.004
-0.003 0.002 0.000
0.006 0.002 0.005

atensor 20 H
-0.397 0.936 -0.871
0.936 -0.359 -0.861
-0.871 -0.861 -0.516
0.003 -0.003 0.001
-0.002 0.001 0.002
0.002 0.003 0.002

atensor 21 H
-0.195 0.809 -2.294
0.809 -1.497 -1.008
-2.294 -1.008 1.210
0.003 -0.004 0.006
0.001 0.009 -0.001
0.012 0.009 -0.007

atensor 22 H
1.623 1.093 -1.450
1.093 -1.080 -0.536
-1.450 -0.536 -0.745
-0.001 -0.006 0.004
-0.002 0.006 0.001
0.008 0.004 0.005

atensor 23 C
0.806 0.541 0.475
0.541 0.096 0.258
0.475 0.258 0.086

0.002 -0.004 -0.003
-0.003 0.002 0.001
-0.005 -0.001 0.008

atensor 24 C
-0.084 -0.014 0.006
-0.014 0.563 0.859
0.006 0.859 1.012
0.012 -0.002 0.001
-0.003 0.001 -0.003
0.000 -0.006 0.000

atensor 25 H
0.161 0.222 0.136
0.222 1.833 1.385
0.136 1.385 1.333
0.002 0.001 0.002
-0.001 -0.001 -0.004
-0.002 -0.007 0.000

atensor 26 H
-1.668 0.276 0.710
0.276 -0.675 2.051
0.710 2.051 2.738
0.006 -0.006 0.002
-0.004 0.007 -0.005
-0.006 -0.014 -0.016

atensor 27 H
-0.843 -0.816 -1.064
-0.816 0.240 2.076
-1.064 2.076 1.165
0.006 0.002 0.004
0.000 -0.001 -0.007
0.005 -0.013 -0.005

atensor 28 H
1.416 0.635 -0.221
0.635 0.489 -0.103
-0.221 -0.103 -0.079
0.000 -0.006 0.001
0.000 -0.001 0.000
0.000 0.001 0.004

atensor 29 H
0.012 0.278 -0.222
0.278 -2.452 -0.007
-0.222 -0.007 -1.593
-0.004 -0.001 0.001
0.001 0.001 0.000
0.001 0.000 0.002

atensor 30 C
2.176 1.839 0.402
1.839 0.554 0.634
0.402 0.634 0.669
0.039 -0.017 0.005
-0.033 0.008 -0.009
0.004 -0.011 0.068

atensor 31 H
2.162 1.265 0.591
1.265 -1.027 0.227
0.591 0.227 -1.338
-0.003 -0.007 -0.002
-0.003 0.006 -0.001
-0.006 -0.002 0.008

atensor 32 H
1.008 1.217 2.259
1.217 -1.367 0.880
2.259 0.880 -0.127
-0.002 -0.006 -0.007
0.000 0.009 0.000
-0.013 -0.009 -0.001

atensor 33 H
0.002 1.174 0.646
1.174 -0.265 0.555
0.646 0.555 -1.020
0.002 -0.004 0.000
-0.003 0.001 -0.002
-0.002 -0.002 0.003

atensor 34 H
-1.217 2.939 -0.451
2.939 0.556 -0.537
-0.451 -0.537 -3.825
0.010 -0.002 0.002
-0.010 -0.003 0.002
0.002 0.001 0.023

atensor 35 H
0.218 -0.289 -0.110
-0.289 -0.684 0.037
-0.110 0.037 -0.694
-0.002 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 36 H
0.311 -0.380 -0.059
-0.380 0.130 0.036
-0.059 0.036 -0.242
-0.001 0.003 0.000
0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.524 -0.591 -0.011
-0.590 0.562 0.031
-0.011 0.031 -0.769
-0.002 0.002 0.000
0.003 -0.003 0.000
0.000 0.000 0.002

atensor 38 Cr
18.919 2.924 -0.256
2.924 27.671 -0.722
-0.256 -0.722 17.783
2.468 -0.368 0.114
-0.389 2.062 0.091
0.114 0.089 3.227

atensor 39 Cl
6.405 0.149 1.807
0.149 2.872 -4.812
1.807 -4.812 -5.861
0.478 0.039 0.039
0.036 0.257 -0.194
0.007 -0.269 0.345

atensor 40 Cl
4.686 1.073 -4.725

1.073 3.479 4.058
-4.725 4.058 -4.751
0.456 0.103 -0.078
0.083 0.287 0.183
-0.044 0.255 0.336

orbtensor 1 N
-476.717 52.978 48.473
52.978 -550.776 9.150
48.473 9.150 -96.153
338.809 -2.897 -2.009
-2.897 352.351 -0.658
-2.009 -0.658 322.865

orbtensor 2 C
-269.174 25.637 25.237
25.637 -297.860 4.665
25.237 4.665 -71.524
252.707 6.254 -5.689
6.254 251.993 -2.253
-5.689 -2.253 211.419

orbtensor 3 C
-221.782 -47.753 23.591
-47.753 -286.635 14.336
23.591 14.336 -56.591
251.837 4.144 -3.908
4.144 263.164 -1.941
-3.908 -1.941 223.450

orbtensor 4 C
-300.826 -22.109 32.925
-22.109 -230.037 9.026
32.925 9.026 -57.921
256.860 3.386 -5.345
3.386 252.676 -1.695
-5.345 -1.695 217.378

orbtensor 5 C
-287.474 2.731 30.208
2.731 -276.128 7.375
30.208 7.375 -58.341
269.099 0.618 -4.477
0.618 266.808 -1.196
-4.477 -1.196 235.420

orbtensor 6 C
-272.935 19.878 22.096
19.878 -297.281 4.358
22.096 4.358 -100.487
262.956 -4.692 -5.776
-4.692 261.269 -0.921
-5.776 -0.921 218.012

orbtensor 7 C
-295.019 12.549 30.565
12.549 -209.717 3.723
30.565 3.723 -60.387
257.584 -4.214 -5.150
-4.214 251.624 -0.667
-5.150 -0.667 217.485

orbtensor 8 C
-246.524 54.065 23.970
54.065 -271.397 0.788
23.970 0.788 -50.511
253.237 -5.647 -4.158

-5.647 256.063 -0.536
-4.158 -0.536 220.248

orbtensor 9 C
-235.718 -36.206 24.820
-36.206 -289.186 12.879
24.820 12.879 -57.868
252.257 -3.416 -4.248
-3.416 257.500 -0.911
-4.248 -0.911 219.203

orbtensor 10 C
-302.334 -14.720 28.577
-14.720 -249.760 7.612
28.577 7.612 -90.131
269.898 -0.702 -4.435
-0.702 264.953 -0.933
-4.435 -0.933 236.153

orbtensor 11 C
-216.840 33.951 -0.010
33.951 -133.534 -6.969
-0.010 -6.969 -207.647
247.213 -8.374 -1.132
-8.374 240.702 0.930
-1.132 0.930 236.375

orbtensor 12 C
-197.072 20.279 0.960
20.279 -106.125 24.741
0.960 24.741 -235.160
242.584 -2.563 -5.096
-2.563 235.842 -6.480
-5.096 -6.480 244.419

orbtensor 13 C
-226.888 -2.622 14.205
-2.622 -93.565 13.901
14.205 13.901 -218.655
246.530 3.970 -1.974
3.970 232.821 -4.718
-1.974 -4.718 244.525

orbtensor 14 C
-200.225 11.772 -10.794
11.772 -110.423 -37.441
-10.794 -37.441 -227.677
245.230 -0.415 4.863
-0.415 236.799 7.298
4.863 7.298 240.819

orbtensor 15 C
-55.091 1.085 6.840
1.085 -47.047 3.027
6.840 3.027 -48.562
219.310 -0.423 2.591
-0.423 217.992 -4.410
2.591 -4.410 228.223

orbtensor 16 H
3.015 -0.715 0.117
-0.715 2.070 1.344
0.117 1.344 1.421
23.665 0.873 -0.654
0.873 29.131 -6.742
-0.654 -6.742 29.284

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orbtensor 17 H
3.251    0.415   -1.957
0.415    3.393    2.410
-1.957   2.410    2.718
30.306   -0.501    0.409
-0.501   20.822  -2.445
0.409    -2.445   28.872

orbtensor 18 H
5.063    0.272   -0.047
0.272    3.509    2.297
-0.047   2.297   -1.359
21.486   -2.517   -0.462
-2.517   26.516    1.295
-0.462    1.295   30.423

orbtensor 19 C
-52.749  -0.579   -5.730
-0.579  -44.560   2.738
-5.730   2.738  -53.879
226.398   0.802  -6.977
0.802  218.243  -1.354
-6.977  -1.354  223.109

orbtensor 20 H
2.170   -0.590    1.124
-0.590   2.183    0.781
1.124    0.781    2.339
26.844   3.468   -4.088
3.468   28.568  -5.083
-4.088   -5.083   26.661

orbtensor 21 H
2.383   -1.569    3.006
-1.569   4.029    1.005
3.006    1.005    0.335
25.815   2.924   -3.035
2.924   24.799    3.280
-3.035   3.280   28.425

orbtensor 22 H
-1.244   -0.961    1.479
-0.961   3.021    1.134
1.479    1.134    3.626
33.766   -2.051   -0.709
-2.051   22.395   -1.240
-0.709   -1.240   25.983

orbtensor 23 C
-49.979  -0.984    4.807
-0.984  -44.967   -3.251
4.807   -3.251  -56.246
229.602   1.572   5.157
1.572  218.427   1.250
5.157    1.250  219.721

orbtensor 24 C
-58.035  -0.110   -4.313
-0.110  -47.474   -3.119
-4.313   -3.119  -45.176
218.595   0.711   -0.146
0.711  218.645   5.070
-0.146   5.070  228.278

orbtensor 25 H
2.872   -1.055   -0.412
-1.055   1.897   -1.142

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-0.412	-1.142	1.737
24.303	2.638	1.721
2.638	30.031	6.217
1.721	6.217	27.745

orbtensor 26 H

4.672	-0.414	-1.497
-0.414	3.171	-2.584
-1.497	-2.584	-0.630
22.352	-2.619	2.796
-2.619	26.395	-0.370
2.796	-0.370	29.682

orbtensor 27 H

4.187	-0.097	1.604
-0.097	3.055	-2.509
1.604	-2.509	2.124
30.006	0.177	-0.745
0.177	21.199	3.024
-0.745	3.024	28.792

orbtensor 28 H

-5.802	-6.456	0.613
-6.456	-16.862	1.328
0.613	1.328	-2.939
32.111	5.145	-1.293
5.145	41.592	-1.297
-1.293	-1.297	23.751

orbtensor 29 H

-18.555	-2.657	2.289
-2.657	-3.445	0.408
2.289	0.408	-1.956
41.581	2.150	-2.707
2.150	30.595	-0.603
-2.707	-0.603	21.692

orbtensor 30 C

-233.241	-7.976	-9.703
-7.976	-95.958	-20.736
-9.703	-20.736	-209.928
247.284	5.237	0.840
5.237	233.442	4.253
0.840	4.253	243.154

orbtensor 31 H

-1.635	-1.262	0.008
-1.262	2.889	-0.775
0.008	-0.775	4.149
33.639	-1.652	-1.209
-1.652	22.613	1.948
-1.209	1.948	25.892

orbtensor 32 H

0.796	-2.009	-2.987
-2.009	3.907	-0.733
-2.987	-0.733	2.041
27.444	2.237	3.175
2.237	24.322	-3.723
3.175	-3.723	27.270

orbtensor 33 H

1.640	-0.835	-0.876
-0.835	2.089	-0.560
-0.876	-0.560	2.961
28.765	4.875	3.155
4.875	29.179	3.757

3.155 3.757 24.130

orbtensor 34 H

-8.285 3.628 0.872
3.628 -14.522 0.013
0.872 0.013 -0.726
34.865 -1.226 -1.925
-1.226 36.525 -0.426
-1.925 -0.426 19.973

orbtensor 35 H

-18.386 0.594 2.100
0.594 -3.383 -0.030
2.100 -0.030 -2.323
42.103 -0.562 -2.645
-0.562 30.441 -0.236
-2.645 -0.236 21.939

orbtensor 36 H

-8.100 7.726 0.341
7.726 -13.851 -0.638
0.341 -0.638 -3.419
34.019 -6.674 -1.147
-6.674 38.495 0.339
-1.147 0.339 23.525

orbtensor 37 H

-5.282 -5.242 0.636
-5.242 -16.483 1.193
0.636 1.193 -1.904
31.526 1.706 -1.292
1.706 40.212 -0.855
-1.292 -0.855 22.231

orbtensor 38 Cr

-5042.896 442.447 -78.204
442.447 -3681.490 -121.103
-78.204 -121.103 -5513.055
1814.989 0.961 -0.391
0.961 1814.311 -0.197
-0.391 -0.197 1812.293

orbtensor 39 Cl

-319.228 -19.524 15.304
-19.524 -458.010 162.180
15.304 162.180 -392.882
1141.478 -0.666 -2.532
-0.666 1145.000 4.821
-2.532 4.821 1146.531

orbtensor 40 Cl

-330.493 -61.001 -26.082
-61.001 -479.249 -145.433
-26.082 -145.433 -360.306
1143.092 -1.651 3.609
-1.651 1144.366 -4.421
3.609 -4.421 1145.551

gtensor (ppt)

-0.151 0.005 0.000
0.005 -0.152 -0.001
0.000 -0.001 -0.153
-4.178 3.424 -0.910
3.424 -3.206 -0.689
-0.910 -0.689 -10.132

zfstensor (cm-1)

-0.362263 -0.236187 -0.013949
 -0.236187 0.765003 0.071018
 -0.013949 0.071018 -0.402740

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.1013	-36.54033	3840.40760	-2.49544	3837.91216	3801.37182
2	C	3.6580	25.85367	-1921.44804	-1.52721	-1922.97525	-1897.12159
3	C	-0.6177	57.81433	324.44352	-0.52252	323.92101	381.73534
4	C	1.3187	46.04333	-692.65978	-0.41365	-693.07343	-647.03010
5	C	-1.0847	49.79467	569.74594	-0.12863	569.61731	619.41198
6	C	0.4600	23.84467	-241.62551	-0.50613	-242.13163	-218.28696
7	C	0.2350	53.85667	-123.43912	-0.01954	-123.45866	-69.60199
8	C	-0.3427	53.70533	179.99349	0.13011	180.12360	233.82894
9	C	-0.7267	48.72933	381.69826	0.36071	382.05897	430.78831
10	C	0.5837	42.92633	-306.58425	0.92582	-305.65842	-262.73209
11	C	-0.5987	55.42300	314.46334	0.74254	315.20588	370.62888
12	C	1.3800	61.49600	-724.87652	0.95513	-723.92139	-662.42539
13	C	1.1733	61.58933	-616.32013	-2.82514	-619.14527	-557.55594
14	C	1.3803	61.50767	-725.05161	1.67656	-723.37505	-661.86738
15	C	0.5000	171.60833	-262.63642	0.28007	-262.35635	-90.74802
16	H	1.1053	29.52867	-146.02352	0.14040	-145.88312	-116.35445
17	H	0.1873	29.78733	-24.74826	0.27746	-24.47080	5.31654
18	H	0.1297	28.54600	-17.13002	0.03194	-17.09808	11.44792
19	C	0.3333	172.18733	-175.09095	-0.88130	-175.97225	-3.78491
20	H	-0.4220	29.58833	55.74963	-0.33387	55.41576	85.00410
21	H	-0.1590	28.59533	21.00519	-0.55094	20.45425	49.04958
22	H	-0.0640	29.18233	8.45492	-0.73068	7.72424	36.90658
23	C	0.3333	172.18600	-175.09095	-0.81522	-175.90617	-3.72017
24	C	0.5013	171.61100	-263.33678	0.55815	-262.77864	-91.16764
25	H	1.1093	29.52833	-146.55195	0.25589	-146.29606	-116.76773
26	H	0.1307	28.54733	-17.26213	0.18778	-17.07435	11.47298
27	H	0.1873	29.78767	-24.74826	0.45594	-24.29232	5.49535
28	H	0.6097	23.95033	-80.54192	-0.30147	-80.84340	-56.89306
29	H	-1.3447	23.30400	177.64140	-0.40811	177.23329	200.53729
30	C	1.1713	61.58433	-615.26958	-2.59647	-617.86606	-556.28172
31	H	-0.0640	29.18233	8.45492	-0.71671	7.73821	36.92054
32	H	-0.1600	28.59333	21.13730	-0.51234	20.62496	49.21830
33	H	-0.4257	29.58800	56.23403	-0.28856	55.94546	85.53346
34	H	-1.4853	22.61000	196.22461	-0.58577	195.63884	218.24884
35	H	-0.3867	23.46367	51.08181	-0.03924	51.04257	74.50624
36	H	0.0660	23.55633	-8.71914	0.08267	-8.63647	14.91987
37	H	-0.2447	23.43333	32.32246	0.31224	32.63469	56.06803
38	Cr	24.0433	-2931.94933	56081.52936	-7.22775	56074.30161	53142.35227
39	Cl	1.4987	754.29633	-2018.35542	-7.58016	-2025.93558	-1271.63924
40	Cl	1.4977	754.32033	-2017.00865	-3.10038	-2020.10902	-1265.78869

=====
 CrL1-STO-PBE0-No-ZFS
 Temperature: 295
 Spin: 1.5

atensor 1 N
 -2.691 0.204 -0.276
 0.204 -3.458 -0.072
 -0.276 -0.072 -4.724
 -0.011 0.005 0.005
 0.000 0.017 0.000
 0.005 0.000 0.027

atensor 2 C
 3.175 0.964 0.168
 0.964 2.231 -0.039
 0.168 -0.039 4.702

-0.033 0.004 0.005
0.021 -0.006 -0.002
0.004 0.000 0.005

atensor 3 C
0.057 0.196 -0.265
0.196 -0.522 -0.075
-0.265 -0.075 -1.895
-0.001 -0.003 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 4 C
0.587 0.068 0.280
0.068 0.027 0.086
0.280 0.086 2.724
-0.008 0.002 0.001
0.003 -0.006 0.000
0.001 0.000 0.001

atensor 5 C
-0.501 -0.111 -0.165
-0.111 -1.007 -0.013
-0.165 -0.013 -1.776
-0.002 -0.001 0.001
0.001 0.004 0.000
0.001 0.000 0.003

atensor 6 C
1.379 -0.545 -0.080
-0.545 -0.801 0.120
-0.080 0.120 0.626
0.003 0.003 0.000
-0.020 -0.011 0.003
0.001 0.000 0.003

atensor 7 C
0.300 -0.110 0.070
-0.110 0.013 0.042
0.070 0.042 0.798
-0.001 0.002 0.000
-0.001 -0.003 0.000
0.000 0.000 0.001

atensor 8 C
-0.202 -0.161 -0.110
-0.161 -0.274 -0.008
-0.110 -0.008 -1.081
0.000 0.003 0.000
0.001 0.000 0.000
0.000 0.000 0.001

atensor 9 C
-1.059 -0.247 0.103
-0.247 -0.904 0.052
0.103 0.052 -0.342
-0.006 -0.005 0.001
0.005 0.005 -0.001
0.001 0.001 0.001

atensor 10 C
1.437 -1.031 -0.218
-1.031 1.201 0.074
-0.218 0.074 -0.492
-0.003 0.006 0.001
0.006 -0.005 0.000
0.001 0.000 0.007

atensor 11 C
-0.297 -1.666 0.009
-1.666 -2.949 0.294
0.009 0.294 -0.683
0.076 0.029 0.001
-0.018 -0.023 0.006
0.003 0.000 0.092

atensor 12 C
0.038 -0.580 0.028
-0.580 1.817 -2.227
0.028 -2.227 1.297
0.076 -0.001 0.003
0.005 -0.001 0.057
-0.003 0.039 0.060

atensor 13 C
1.733 1.513 -0.871
1.513 -0.530 -0.997
-0.871 -0.997 0.950
0.048 -0.021 0.003
-0.037 0.012 0.029
0.007 0.027 0.076

atensor 14 C
0.105 0.010 0.266
0.010 2.129 2.244
0.266 2.244 0.920
0.075 -0.011 -0.006
-0.009 -0.007 -0.052
0.000 -0.033 0.067

atensor 15 C
-0.097 -0.228 0.291
-0.228 0.404 -0.825
0.291 -0.825 0.972
0.012 0.001 -0.005
-0.001 0.001 0.005
-0.004 0.009 -0.001

atensor 16 H
-0.497 -0.158 0.186
-0.158 1.017 -1.460
0.186 -1.460 0.864
0.004 0.003 -0.004
-0.001 -0.001 0.007
0.000 0.012 -0.002

atensor 17 H
-0.267 -1.296 1.588
-1.296 -0.084 -1.836
1.588 -1.836 0.705
0.004 0.009 -0.012
0.004 0.000 0.011
-0.013 0.019 -0.005

atensor 18 H
-1.947 -0.242 0.528
-0.242 -1.211 -1.894
0.528 -1.894 3.065
0.010 -0.002 -0.010
-0.003 0.010 0.007
-0.002 0.021 -0.028

atensor 19 C
0.640 0.445 -0.632

0.445 0.169 -0.397
-0.632 -0.398 0.515
0.004 -0.004 0.005
-0.003 0.003 0.000
0.008 0.004 0.005

atensor 20 H
-0.967 0.977 -0.878
0.977 -0.910 -0.900
-0.878 -0.900 -1.087
0.003 -0.005 0.003
-0.004 0.003 0.004
0.005 0.007 0.002

atensor 21 H
-0.424 0.825 -2.399
0.825 -1.849 -1.074
-2.399 -1.074 1.070
0.004 -0.007 0.012
0.000 0.012 -0.001
0.021 0.013 -0.012

atensor 22 H
1.643 1.162 -1.504
1.162 -1.172 -0.575
-1.504 -0.575 -0.805
-0.005 -0.010 0.008
-0.003 0.009 0.001
0.013 0.006 0.008

atensor 23 C
0.934 0.573 0.479
0.572 0.215 0.275
0.479 0.275 0.174
0.001 -0.005 -0.004
-0.004 0.003 0.001
-0.007 -0.002 0.008

atensor 24 C
-0.170 -0.015 0.003
-0.015 0.524 0.892
0.003 0.892 0.929
0.013 -0.001 0.002
-0.002 0.000 -0.005
0.001 -0.009 -0.001

atensor 25 H
-0.500 0.216 0.146
0.216 1.221 1.430
0.146 1.430 0.676
0.005 0.000 0.002
-0.003 -0.003 -0.007
-0.002 -0.013 -0.001

atensor 26 H
-1.884 0.294 0.742
0.294 -0.929 2.166
0.742 2.166 2.724
0.011 -0.007 0.000
-0.006 0.008 -0.008
-0.008 -0.022 -0.027

atensor 27 H
-0.972 -0.870 -1.106
-0.870 0.191 2.180
-1.106 2.180 1.136
0.009 0.004 0.008

0.002 -0.002 -0.012
0.010 -0.021 -0.009

atensor 28 H
1.423 0.610 -0.214
0.610 0.415 -0.096
-0.214 -0.096 -0.027
-0.002 -0.006 0.001
-0.001 0.001 0.000
0.001 0.001 0.006

atensor 29 H
0.185 0.223 -0.193
0.223 -1.727 -0.012
-0.193 -0.012 -1.212
-0.005 -0.002 0.001
0.002 0.002 0.000
0.001 0.000 0.003

atensor 30 C
2.081 1.773 0.441
1.773 -0.421 0.650
0.441 0.650 0.487
0.048 -0.027 0.007
-0.043 0.009 -0.014
0.004 -0.016 0.079

atensor 31 H
2.202 1.345 0.614
1.345 -1.114 0.248
0.614 0.248 -1.422
-0.010 -0.012 -0.003
-0.003 0.008 0.000
-0.008 -0.003 0.012

atensor 32 H
0.835 1.258 2.370
1.258 -1.711 0.951
2.370 0.951 -0.334
-0.006 -0.011 -0.013
-0.001 0.011 0.000
-0.023 -0.012 -0.002

atensor 33 H
-0.566 1.224 0.648
1.224 -0.812 0.580
0.648 0.580 -1.598
0.001 -0.007 -0.002
-0.005 0.002 -0.002
-0.005 -0.005 0.005

atensor 34 H
-0.863 3.459 -0.503
3.459 1.024 -0.618
-0.503 -0.618 -3.721
0.009 -0.019 0.004
-0.015 -0.005 0.003
0.004 0.004 0.033

atensor 35 H
0.200 -0.266 -0.106
-0.266 -0.719 0.036
-0.106 0.036 -0.677
-0.003 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.003

atensor 36 H
0.473 -0.315 -0.063
-0.315 0.250 0.029
-0.063 0.029 -0.093
-0.002 0.003 0.001
0.002 -0.001 0.000
0.001 0.000 0.003

atensor 37 H
-0.523 -0.640 -0.008
-0.640 0.575 0.037
-0.008 0.037 -0.755
-0.001 0.005 0.001
0.004 -0.004 0.000
0.001 0.000 0.005

atensor 38 Cr
27.532 3.238 -0.352
3.238 37.357 -0.823
-0.352 -0.823 25.748
3.226 -0.510 0.136
-0.560 2.389 0.133
0.138 0.126 4.114

atensor 39 Cl
5.973 0.353 1.529
0.353 2.414 -5.016
1.529 -5.016 -5.027
0.448 0.026 0.041
0.001 0.199 -0.118
0.015 -0.279 0.276

atensor 40 Cl
4.470 1.360 -4.190
1.360 3.050 4.278
-4.190 4.278 -4.162
0.422 0.093 -0.088
0.030 0.226 0.118
-0.058 0.268 0.275

orbtensor 1 N
-465.826 40.995 54.696
40.995 -540.394 12.315
54.696 12.315 -40.984
322.133 -3.100 -4.225
-3.100 333.204 -1.141
-4.225 -1.141 289.376

orbtensor 2 C
-285.207 28.244 25.990
28.244 -322.637 4.866
25.990 4.866 -80.648
260.136 6.594 -4.528
6.594 262.108 -2.076
-4.528 -2.076 227.710

orbtensor 3 C
-231.869 -41.946 26.032
-41.946 -275.843 13.551
26.032 13.551 -46.905
258.918 -1.447 -5.031
-1.447 255.288 -1.047
-5.031 -1.047 220.502

orbtensor 4 C
-306.387 -24.935 33.746
-24.935 -249.549 10.077

33.746	10.077	-58.245
252.944	3.148	-4.039
3.148	263.832	-1.842
-4.039	-1.842	223.289

orbtensor 5 C

-290.001	2.554	32.248
2.554	-270.313	7.671
32.248	7.671	-45.024
271.201	1.352	-5.529
1.352	260.787	-1.283
-5.529	-1.283	229.757

orbtensor 6 C

-283.833	13.327	23.429
13.327	-313.082	5.626
23.429	5.626	-103.775
270.390	0.826	-4.976
0.826	269.107	-1.387
-4.976	-1.387	232.985

orbtensor 7 C

-297.243	15.804	30.698
15.804	-222.259	3.713
30.698	3.713	-61.036
255.003	-5.186	-4.140
-5.186	261.765	-0.723
-4.140	-0.723	222.290

orbtensor 8 C

-257.510	45.855	25.656
45.855	-273.720	1.898
25.656	1.898	-51.053
259.853	2.768	-4.697
2.768	257.513	-1.514
-4.697	-1.514	225.076

orbtensor 9 C

-248.216	-35.315	26.704
-35.315	-289.633	12.811
26.704	12.811	-55.736
260.060	-6.018	-4.951
-6.018	254.939	-0.425
-4.951	-0.425	220.962

orbtensor 10 C

-302.572	-19.249	30.154
-19.249	-245.676	8.351
30.154	8.351	-79.855
268.160	1.729	-5.139
1.729	262.428	-1.388
-5.139	-1.388	229.740

orbtensor 11 C

-226.956	30.235	0.465
30.235	-117.122	-7.435
0.465	-7.435	-214.998
258.620	-3.679	-0.641
-3.679	231.288	1.212
-0.641	1.212	252.741

orbtensor 12 C

-209.732	24.849	0.752
24.849	-101.383	24.787
0.752	24.787	-238.483
262.517	-4.313	-4.667
-4.313	237.650	-2.430

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-4.667   -2.430   256.274

orbtensor 13 C
-242.142   2.755   10.658
2.755  -89.200   12.377
10.658   12.377  -232.705
261.266  -1.035   3.416
-1.035   235.952  -1.325
3.416   -1.325   259.940

orbtensor 14 C
-212.214   16.223  -8.596
16.223  -105.678  -39.285
-8.596  -39.285  -231.504
264.471  -3.138   2.712
-3.138   238.136   4.572
2.712    4.572   253.838

orbtensor 15 C
-49.477   2.379   3.677
2.379  -41.803   3.410
3.677   3.410  -47.606
219.778  -1.290   4.755
-1.290   217.154  -4.212
4.755   -4.212   231.465

orbtensor 16 H
3.289   -0.797  -0.313
-0.797   2.490   1.603
-0.313   1.603   1.239
23.489   1.114  -0.395
1.114   29.060  -7.041
-0.395  -7.041   29.600

orbtensor 17 H
2.262   0.461  -2.778
0.461   3.343   2.366
-2.778   2.366   2.117
31.780  -0.725   1.070
-0.725   20.804  -2.182
1.070   -2.182   29.518

orbtensor 18 H
5.341   0.370  -0.624
0.370   4.225   1.671
-0.624   1.671  -2.776
21.538  -2.704  -0.275
-2.704   26.010   2.243
-0.275   2.243   31.627

orbtensor 19 C
-47.634  -1.761  -2.607
-1.761  -38.104   2.049
-2.607   2.049  -49.935
226.746   1.485  -9.280
1.485   216.414  -0.230
-9.280  -0.230   224.117

orbtensor 20 H
2.693   -0.748   1.557
-0.748   2.740   0.843
1.557   0.843   2.515
26.614   3.572  -4.538
3.572   28.598  -5.151
-4.538  -5.151   26.747

orbtensor 21 H

```

2.481	-1.392	3.634
-1.392	4.632	0.375
3.634	0.375	-0.837
25.849	2.617	-3.365
2.617	24.454	4.055
-3.365	4.055	29.648

orbtensor 22 H

-1.859	-0.803	2.055
-0.803	3.042	0.859
2.055	0.859	3.704
34.820	-2.287	-1.064
-2.287	22.347	-0.830
-1.064	-0.830	26.031

orbtensor 23 C

-46.463	-2.129	1.848
-2.129	-38.332	-2.298
1.848	-2.298	-50.812
231.123	2.120	7.302
2.120	216.445	0.129
7.302	0.129	219.710

orbtensor 24 C

-51.204	1.180	-2.767
1.180	-42.372	-4.121
-2.767	-4.121	-45.369
218.199	-0.253	-1.282
-0.253	217.814	5.422
-1.282	5.422	232.384

orbtensor 25 H

3.316	-1.188	-0.130
-1.188	2.230	-1.397
-0.130	-1.397	1.405
24.026	2.938	1.594
2.938	29.998	6.474
1.594	6.474	28.125

orbtensor 26 H

5.111	-0.153	-1.426
-0.153	3.906	-2.181
-1.426	-2.181	-2.292
22.396	-3.027	2.953
-3.027	25.771	-1.112
2.953	-1.112	31.013

orbtensor 27 H

3.604	-0.003	2.408
-0.003	2.953	-2.534
2.408	-2.534	1.093
31.108	-0.148	-1.503
-0.148	21.152	2.893
-1.503	2.893	29.841

orbtensor 28 H

-4.461	-6.863	0.607
-6.863	-15.872	1.385
0.607	1.385	-1.792
30.800	5.507	-1.375
5.507	40.792	-1.381
-1.375	-1.381	21.920

orbtensor 29 H

-19.108	-3.533	2.267
-3.533	-2.635	0.451
2.267	0.451	-2.880

41.758	2.987	-2.768
2.987	29.912	-0.690
-2.768	-0.690	21.639

orbtensor 30 C

-246.753	-2.334	-6.703
-2.334	-91.692	-22.064
-6.703	-22.064	-225.725
259.506	-0.680	-3.277
-0.680	236.262	3.239
-3.277	3.239	261.385

orbtensor 31 H

-2.485	-1.072	-0.332
-1.072	2.896	-0.516
-0.332	-0.516	4.431
34.809	-1.970	-1.122
-1.970	22.514	1.614
-1.122	1.614	25.875

orbtensor 32 H

0.479	-1.755	-3.869
-1.755	4.577	-0.271
-3.869	-0.271	1.191
27.727	1.787	3.794
1.787	23.885	-4.293
3.794	-4.293	28.338

orbtensor 33 H

1.922	-1.026	-1.317
-1.026	2.597	-0.573
-1.317	-0.573	3.374
28.774	5.023	3.615
5.023	29.215	3.788
3.615	3.788	23.968

orbtensor 34 H

-6.864	5.990	0.646
5.990	-14.290	-0.296
0.646	-0.296	-0.284
33.769	-3.196	-1.855
-3.196	36.233	-0.198
-1.855	-0.198	18.868

orbtensor 35 H

-19.144	0.810	2.120
0.810	-2.549	-0.101
2.120	-0.101	-2.864
42.791	-0.778	-2.735
-0.778	29.778	-0.187
-2.735	-0.187	21.878

orbtensor 36 H

-7.293	8.185	0.315
8.185	-13.588	-0.684
0.315	-0.684	-2.704
33.332	-7.006	-1.208
-7.006	38.302	0.346
-1.208	0.346	22.291

orbtensor 37 H

-4.414	-6.242	0.636
-6.242	-16.545	1.346
0.636	1.346	-1.245
30.874	2.457	-1.397
2.457	40.280	-0.998
-1.397	-0.998	20.989

```

orbtensor 38 Cr
-5274.634  696.832 -130.654
696.832 -3606.590 -176.344
-130.654 -176.344 -6071.342
1808.932  2.168 -0.457
2.168 1816.270 -0.636
-0.457 -0.636 1806.071

```

```

orbtensor 39 Cl
-120.577 -17.336  22.186
-17.336 -248.416  64.643
22.186  64.643 -207.984
1141.011 -0.627 -2.175
-0.627 1145.461  5.274
-2.175  5.274 1145.830

```

```

orbtensor 40 Cl
-136.512 -34.870 -38.115
-34.870 -256.467 -54.023
-38.115 -54.023 -183.657
1142.434 -1.764  3.251
-1.764 1144.759 -4.934
3.251 -4.934 1145.107

```

```

gtensor (ppt)
-0.163  0.006  0.000
0.006 -0.149 -0.001
0.000 -0.001 -0.163
-10.358  4.307 -1.154
4.307 -7.461 -0.927
-1.154 -0.927 -17.910

```

```

averaging
2H Average:34
4H Average:29
9,10H Average:16,17,18,20,21,22
5H Average:35
8,11H Average:25,26,27,31,32,33
6H Average:36
3H Average:28
7H Average:37

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.6133	-34.16367	6583.65231	-3.42571	6580.22660	6546.06294
2	C	3.3580	20.48733	-1758.49899	0.47242	-1758.02657	-1737.53924
3	C	-0.7863	60.03033	411.78272	-1.01388	410.76884	470.79917
4	C	1.1083	41.96133	-580.40591	1.36597	-579.03994	-537.07861
5	C	-1.0930	52.13567	572.37624	-0.42472	571.95152	624.08718
6	C	0.3997	23.93067	-209.29524	0.88370	-208.41155	-184.48088
7	C	0.3693	52.84000	-193.41045	0.48019	-192.93026	-140.09026
8	C	-0.5187	53.38633	271.61251	-0.33755	271.27496	324.66130
9	C	-0.7683	47.45867	402.35658	0.53280	402.88938	450.34804
10	C	0.7150	44.07500	-374.42727	-0.17405	-374.60132	-330.52632
11	C	-1.2613	61.19100	660.52811	2.18760	662.71571	723.90671
12	C	1.0957	68.94767	-573.77270	0.07744	-573.69526	-504.74760
13	C	0.7630	64.37033	-399.56365	-0.95451	-400.51816	-336.14783
14	C	1.0963	69.01633	-574.12182	0.07732	-574.04450	-505.02816
15	C	0.4303	176.50367	-225.35460	0.46192	-224.89268	-48.38901
16	H	0.4617	29.72233	-60.80434	0.01095	-60.79338	-31.07105
17	H	0.1177	29.94133	-15.49742	0.36098	-15.13645	14.80489
18	H	-0.0337	28.65500	4.43411	0.58262	5.01672	33.67172
19	C	0.4453	177.20133	-233.20971	-0.40578	-233.61549	-56.41416
20	H	-0.9853	29.96900	129.77445	-0.28780	129.48666	159.45566

21	H	-0.3997	28.74233	52.63856	0.01379	52.65234	81.39468
22	H	-0.1073	29.36167	14.13646	-0.36640	13.77006	43.13173
23	C	0.4450	177.22367	-233.03516	-0.40544	-233.44059	-56.21692
24	C	0.4317	176.48400	-226.05283	0.46263	-225.59019	-49.10619
25	H	0.4660	29.70000	-61.37506	0.01128	-61.36378	-31.66378
26	H	-0.0323	28.63500	4.25850	0.58266	4.84116	33.47616
27	H	0.1177	29.91700	-15.49742	0.36126	-15.13617	14.78083
28	H	0.6053	23.79567	-79.72612	-0.22234	-79.94846	-56.15279
29	H	-0.9180	22.89533	120.90624	-0.04936	120.85688	143.75222
30	C	0.7610	64.32767	-398.51630	-0.95082	-399.46712	-335.13946
31	H	-0.1080	29.34667	14.22426	-0.36624	13.85803	43.20469
32	H	-0.4023	28.73233	52.98977	0.01458	53.00435	81.73669
33	H	-0.9893	29.95000	130.30128	-0.28742	130.01386	159.96386
34	H	-1.1743	22.47733	154.66691	-1.26508	153.40184	175.87917
35	H	-0.3987	23.29667	52.50685	0.02125	52.52810	75.82477
36	H	0.2100	23.44667	-27.65829	0.00501	-27.65328	-4.20661
37	H	-0.2343	23.31300	30.86314	-0.01554	30.84760	54.16060
38	Cr	33.4553	-3173.76433	77797.74725	27.47640	77825.22365	74651.45931
39	Cl	1.4277	951.77500	-1916.88432	-13.34804	-1930.23236	-978.45736
40	Cl	1.4270	951.88800	-1915.98921	-13.33875	-1929.32796	-977.43996

=====
CrL1-STO-PBE0-ORCA

Temperature: 295

Spin: 1.5

atensor 1 N

-2.691 0.204 -0.276
0.204 -3.458 -0.072
-0.276 -0.072 -4.724
-0.011 0.005 0.005
0.000 0.017 0.000
0.005 0.000 0.027

atensor 2 C

3.175 0.964 0.168
0.964 2.231 -0.039
0.168 -0.039 4.702
-0.033 0.004 0.005
0.021 -0.006 -0.002
0.004 0.000 0.005

atensor 3 C

0.057 0.196 -0.265
0.196 -0.522 -0.075
-0.265 -0.075 -1.895
-0.001 -0.003 0.000
0.001 0.000 0.000
0.000 0.000 0.002

atensor 4 C

0.587 0.068 0.280
0.068 0.027 0.086
0.280 0.086 2.724
-0.008 0.002 0.001
0.003 -0.006 0.000
0.001 0.000 0.001

atensor 5 C

-0.501 -0.111 -0.165
-0.111 -1.007 -0.013
-0.165 -0.013 -1.776
-0.002 -0.001 0.001
0.001 0.004 0.000
0.001 0.000 0.003

atensor 6 C
1.379 -0.545 -0.080
-0.545 -0.801 0.120
-0.080 0.120 0.626
0.003 0.003 0.000
-0.020 -0.011 0.003
0.001 0.000 0.003

atensor 7 C
0.300 -0.110 0.070
-0.110 0.013 0.042
0.070 0.042 0.798
-0.001 0.002 0.000
-0.001 -0.003 0.000
0.000 0.000 0.001

atensor 8 C
-0.202 -0.161 -0.110
-0.161 -0.274 -0.008
-0.110 -0.008 -1.081
0.000 0.003 0.000
0.001 0.000 0.000
0.000 0.000 0.001

atensor 9 C
-1.059 -0.247 0.103
-0.247 -0.904 0.052
0.103 0.052 -0.342
-0.006 -0.005 0.001
0.005 0.005 -0.001
0.001 0.001 0.001

atensor 10 C
1.437 -1.031 -0.218
-1.031 1.201 0.074
-0.218 0.074 -0.492
-0.003 0.006 0.001
0.006 -0.005 0.000
0.001 0.000 0.007

atensor 11 C
-0.297 -1.666 0.009
-1.666 -2.949 0.294
0.009 0.294 -0.683
0.076 0.029 0.001
-0.018 -0.023 0.006
0.003 0.000 0.092

atensor 12 C
0.038 -0.580 0.028
-0.580 1.817 -2.227
0.028 -2.227 1.297
0.076 -0.001 0.003
0.005 -0.001 0.057
-0.003 0.039 0.060

atensor 13 C
1.733 1.513 -0.871
1.513 -0.530 -0.997
-0.871 -0.997 0.950
0.048 -0.021 0.003
-0.037 0.012 0.029
0.007 0.027 0.076

atensor 14 C
0.105 0.010 0.266
0.010 2.129 2.244

0.266 2.244 0.920
0.075 -0.011 -0.006
-0.009 -0.007 -0.052
0.000 -0.033 0.067

atensor 15 C
-0.097 -0.228 0.291
-0.228 0.404 -0.825
0.291 -0.825 0.972
0.012 0.001 -0.005
-0.001 0.001 0.005
-0.004 0.009 -0.001

atensor 16 H
-0.497 -0.158 0.186
-0.158 1.017 -1.460
0.186 -1.460 0.864
0.004 0.003 -0.004
-0.001 -0.001 0.007
0.000 0.012 -0.002

atensor 17 H
-0.267 -1.296 1.588
-1.296 -0.084 -1.836
1.588 -1.836 0.705
0.004 0.009 -0.012
0.004 0.000 0.011
-0.013 0.019 -0.005

atensor 18 H
-1.947 -0.242 0.528
-0.242 -1.211 -1.894
0.528 -1.894 3.065
0.010 -0.002 -0.010
-0.003 0.010 0.007
-0.002 0.021 -0.028

atensor 19 C
0.640 0.445 -0.632
0.445 0.169 -0.397
-0.632 -0.398 0.515
0.004 -0.004 0.005
-0.003 0.003 0.000
0.008 0.004 0.005

atensor 20 H
-0.967 0.977 -0.878
0.977 -0.910 -0.900
-0.878 -0.900 -1.087
0.003 -0.005 0.003
-0.004 0.003 0.004
0.005 0.007 0.002

atensor 21 H
-0.424 0.825 -2.399
0.825 -1.849 -1.074
-2.399 -1.074 1.070
0.004 -0.007 0.012
0.000 0.012 -0.001
0.021 0.013 -0.012

atensor 22 H
1.643 1.162 -1.504
1.162 -1.172 -0.575
-1.504 -0.575 -0.805
-0.005 -0.010 0.008
-0.003 0.009 0.001

0.013 0.006 0.008

atensor 23 C
0.934 0.573 0.479
0.572 0.215 0.275
0.479 0.275 0.174
0.001 -0.005 -0.004
-0.004 0.003 0.001
-0.007 -0.002 0.008

atensor 24 C
-0.170 -0.015 0.003
-0.015 0.524 0.892
0.003 0.892 0.929
0.013 -0.001 0.002
-0.002 0.000 -0.005
0.001 -0.009 -0.001

atensor 25 H
-0.500 0.216 0.146
0.216 1.221 1.430
0.146 1.430 0.676
0.005 0.000 0.002
-0.003 -0.003 -0.007
-0.002 -0.013 -0.001

atensor 26 H
-1.884 0.294 0.742
0.294 -0.929 2.166
0.742 2.166 2.724
0.011 -0.007 0.000
-0.006 0.008 -0.008
-0.008 -0.022 -0.027

atensor 27 H
-0.972 -0.870 -1.106
-0.870 0.191 2.180
-1.106 2.180 1.136
0.009 0.004 0.008
0.002 -0.002 -0.012
0.010 -0.021 -0.009

atensor 28 H
1.423 0.610 -0.214
0.610 0.415 -0.096
-0.214 -0.096 -0.027
-0.002 -0.006 0.001
-0.001 0.001 0.000
0.001 0.001 0.006

atensor 29 H
0.185 0.223 -0.193
0.223 -1.727 -0.012
-0.193 -0.012 -1.212
-0.005 -0.002 0.001
0.002 0.002 0.000
0.001 0.000 0.003

atensor 30 C
2.081 1.773 0.441
1.773 -0.421 0.650
0.441 0.650 0.487
0.048 -0.027 0.007
-0.043 0.009 -0.014
0.004 -0.016 0.079

atensor 31 H

2.202 1.345 0.614
1.345 -1.114 0.248
0.614 0.248 -1.422
-0.010 -0.012 -0.003
-0.003 0.008 0.000
-0.008 -0.003 0.012

atensor 32 H
0.835 1.258 2.370
1.258 -1.711 0.951
2.370 0.951 -0.334
-0.006 -0.011 -0.013
-0.001 0.011 0.000
-0.023 -0.012 -0.002

atensor 33 H
-0.566 1.224 0.648
1.224 -0.812 0.580
0.648 0.580 -1.598
0.001 -0.007 -0.002
-0.005 0.002 -0.002
-0.005 -0.005 0.005

atensor 34 H
-0.863 3.459 -0.503
3.459 1.024 -0.618
-0.503 -0.618 -3.721
0.009 -0.019 0.004
-0.015 -0.005 0.003
0.004 0.004 0.033

atensor 35 H
0.200 -0.266 -0.106
-0.266 -0.719 0.036
-0.106 0.036 -0.677
-0.003 0.001 0.001
0.001 0.000 0.000
0.001 0.000 0.003

atensor 36 H
0.473 -0.315 -0.063
-0.315 0.250 0.029
-0.063 0.029 -0.093
-0.002 0.003 0.001
0.002 -0.001 0.000
0.001 0.000 0.003

atensor 37 H
-0.523 -0.640 -0.008
-0.640 0.575 0.037
-0.008 0.037 -0.755
-0.001 0.005 0.001
0.004 -0.004 0.000
0.001 0.000 0.005

atensor 38 Cr
27.532 3.238 -0.352
3.238 37.357 -0.823
-0.352 -0.823 25.748
3.226 -0.510 0.136
-0.560 2.389 0.133
0.138 0.126 4.114

atensor 39 Cl
5.973 0.353 1.529
0.353 2.414 -5.016
1.529 -5.016 -5.027

0.448 0.026 0.041
0.001 0.199 -0.118
0.015 -0.279 0.276

atensor 40 C1
4.470 1.360 -4.190
1.360 3.050 4.278
-4.190 4.278 -4.162
0.422 0.093 -0.088
0.030 0.226 0.118
-0.058 0.268 0.275

orbtensor 1 N
-465.826 40.995 54.696
40.995 -540.394 12.315
54.696 12.315 -40.984
322.133 -3.100 -4.225
-3.100 333.204 -1.141
-4.225 -1.141 289.376

orbtensor 2 C
-285.207 28.244 25.990
28.244 -322.637 4.866
25.990 4.866 -80.648
260.136 6.594 -4.528
6.594 262.108 -2.076
-4.528 -2.076 227.710

orbtensor 3 C
-231.869 -41.946 26.032
-41.946 -275.843 13.551
26.032 13.551 -46.905
258.918 -1.447 -5.031
-1.447 255.288 -1.047
-5.031 -1.047 220.502

orbtensor 4 C
-306.387 -24.935 33.746
-24.935 -249.549 10.077
33.746 10.077 -58.245
252.944 3.148 -4.039
3.148 263.832 -1.842
-4.039 -1.842 223.289

orbtensor 5 C
-290.001 2.554 32.248
2.554 -270.313 7.671
32.248 7.671 -45.024
271.201 1.352 -5.529
1.352 260.787 -1.283
-5.529 -1.283 229.757

orbtensor 6 C
-283.833 13.327 23.429
13.327 -313.082 5.626
23.429 5.626 -103.775
270.390 0.826 -4.976
0.826 269.107 -1.387
-4.976 -1.387 232.985

orbtensor 7 C
-297.243 15.804 30.698
15.804 -222.259 3.713
30.698 3.713 -61.036
255.003 -5.186 -4.140
-5.186 261.765 -0.723
-4.140 -0.723 222.290

orbtensor 8 C
-257.510 45.855 25.656
45.855 -273.720 1.898
25.656 1.898 -51.053
259.853 2.768 -4.697
2.768 257.513 -1.514
-4.697 -1.514 225.076

orbtensor 9 C
-248.216 -35.315 26.704
-35.315 -289.633 12.811
26.704 12.811 -55.736
260.060 -6.018 -4.951
-6.018 254.939 -0.425
-4.951 -0.425 220.962

orbtensor 10 C
-302.572 -19.249 30.154
-19.249 -245.676 8.351
30.154 8.351 -79.855
268.160 1.729 -5.139
1.729 262.428 -1.388
-5.139 -1.388 229.740

orbtensor 11 C
-226.956 30.235 0.465
30.235 -117.122 -7.435
0.465 -7.435 -214.998
258.620 -3.679 -0.641
-3.679 231.288 1.212
-0.641 1.212 252.741

orbtensor 12 C
-209.732 24.849 0.752
24.849 -101.383 24.787
0.752 24.787 -238.483
262.517 -4.313 -4.667
-4.313 237.650 -2.430
-4.667 -2.430 256.274

orbtensor 13 C
-242.142 2.755 10.658
2.755 -89.200 12.377
10.658 12.377 -232.705
261.266 -1.035 3.416
-1.035 235.952 -1.325
3.416 -1.325 259.940

orbtensor 14 C
-212.214 16.223 -8.596
16.223 -105.678 -39.285
-8.596 -39.285 -231.504
264.471 -3.138 2.712
-3.138 238.136 4.572
2.712 4.572 253.838

orbtensor 15 C
-49.477 2.379 3.677
2.379 -41.803 3.410
3.677 3.410 -47.606
219.778 -1.290 4.755
-1.290 217.154 -4.212
4.755 -4.212 231.465

orbtensor 16 H
3.289 -0.797 -0.313

-0.797	2.490	1.603
-0.313	1.603	1.239
23.489	1.114	-0.395
1.114	29.060	-7.041
-0.395	-7.041	29.600

orbtensor 17 H

2.262	0.461	-2.778
0.461	3.343	2.366
-2.778	2.366	2.117
31.780	-0.725	1.070
-0.725	20.804	-2.182
1.070	-2.182	29.518

orbtensor 18 H

5.341	0.370	-0.624
0.370	4.225	1.671
-0.624	1.671	-2.776
21.538	-2.704	-0.275
-2.704	26.010	2.243
-0.275	2.243	31.627

orbtensor 19 C

-47.634	-1.761	-2.607
-1.761	-38.104	2.049
-2.607	2.049	-49.935
226.746	1.485	-9.280
1.485	216.414	-0.230
-9.280	-0.230	224.117

orbtensor 20 H

2.693	-0.748	1.557
-0.748	2.740	0.843
1.557	0.843	2.515
26.614	3.572	-4.538
3.572	28.598	-5.151
-4.538	-5.151	26.747

orbtensor 21 H

2.481	-1.392	3.634
-1.392	4.632	0.375
3.634	0.375	-0.837
25.849	2.617	-3.365
2.617	24.454	4.055
-3.365	4.055	29.648

orbtensor 22 H

-1.859	-0.803	2.055
-0.803	3.042	0.859
2.055	0.859	3.704
34.820	-2.287	-1.064
-2.287	22.347	-0.830
-1.064	-0.830	26.031

orbtensor 23 C

-46.463	-2.129	1.848
-2.129	-38.332	-2.298
1.848	-2.298	-50.812
231.123	2.120	7.302
2.120	216.445	0.129
7.302	0.129	219.710

orbtensor 24 C

-51.204	1.180	-2.767
1.180	-42.372	-4.121
-2.767	-4.121	-45.369
218.199	-0.253	-1.282

-0.253	217.814	5.422
-1.282	5.422	232.384

orbtensor 25 H

3.316	-1.188	-0.130
-1.188	2.230	-1.397
-0.130	-1.397	1.405
24.026	2.938	1.594
2.938	29.998	6.474
1.594	6.474	28.125

orbtensor 26 H

5.111	-0.153	-1.426
-0.153	3.906	-2.181
-1.426	-2.181	-2.292
22.396	-3.027	2.953
-3.027	25.771	-1.112
2.953	-1.112	31.013

orbtensor 27 H

3.604	-0.003	2.408
-0.003	2.953	-2.534
2.408	-2.534	1.093
31.108	-0.148	-1.503
-0.148	21.152	2.893
-1.503	2.893	29.841

orbtensor 28 H

-4.461	-6.863	0.607
-6.863	-15.872	1.385
0.607	1.385	-1.792
30.800	5.507	-1.375
5.507	40.792	-1.381
-1.375	-1.381	21.920

orbtensor 29 H

-19.108	-3.533	2.267
-3.533	-2.635	0.451
2.267	0.451	-2.880
41.758	2.987	-2.768
2.987	29.912	-0.690
-2.768	-0.690	21.639

orbtensor 30 C

-246.753	-2.334	-6.703
-2.334	-91.692	-22.064
-6.703	-22.064	-225.725
259.506	-0.680	-3.277
-0.680	236.262	3.239
-3.277	3.239	261.385

orbtensor 31 H

-2.485	-1.072	-0.332
-1.072	2.896	-0.516
-0.332	-0.516	4.431
34.809	-1.970	-1.122
-1.970	22.514	1.614
-1.122	1.614	25.875

orbtensor 32 H

0.479	-1.755	-3.869
-1.755	4.577	-0.271
-3.869	-0.271	1.191
27.727	1.787	3.794
1.787	23.885	-4.293
3.794	-4.293	28.338

orbtensor 33 H
1.922 -1.026 -1.317
-1.026 2.597 -0.573
-1.317 -0.573 3.374
28.774 5.023 3.615
5.023 29.215 3.788
3.615 3.788 23.968

orbtensor 34 H
-6.864 5.990 0.646
5.990 -14.290 -0.296
0.646 -0.296 -0.284
33.769 -3.196 -1.855
-3.196 36.233 -0.198
-1.855 -0.198 18.868

orbtensor 35 H
-19.144 0.810 2.120
0.810 -2.549 -0.101
2.120 -0.101 -2.864
42.791 -0.778 -2.735
-0.778 29.778 -0.187
-2.735 -0.187 21.878

orbtensor 36 H
-7.293 8.185 0.315
8.185 -13.588 -0.684
0.315 -0.684 -2.704
33.332 -7.006 -1.208
-7.006 38.302 0.346
-1.208 0.346 22.291

orbtensor 37 H
-4.414 -6.242 0.636
-6.242 -16.545 1.346
0.636 1.346 -1.245
30.874 2.457 -1.397
2.457 40.280 -0.998
-1.397 -0.998 20.989

orbtensor 38 Cr
-5274.634 696.832 -130.654
696.832 -3606.590 -176.344
-130.654 -176.344 -6071.342
1808.932 2.168 -0.457
2.168 1816.270 -0.636
-0.457 -0.636 1806.071

orbtensor 39 Cl
-120.577 -17.336 22.186
-17.336 -248.416 64.643
22.186 64.643 -207.984
1141.011 -0.627 -2.175
-0.627 1145.461 5.274
-2.175 5.274 1145.830

orbtensor 40 Cl
-136.512 -34.870 -38.115
-34.870 -256.467 -54.023
-38.115 -54.023 -183.657
1142.434 -1.764 3.251
-1.764 1144.759 -4.934
3.251 -4.934 1145.107

gtensor (ppt)
-0.163 0.006 0.000
0.006 -0.149 -0.001

```

0.000   -0.001   -0.163
-10.358  4.307   -1.154
4.307   -7.461   -0.927
-1.154   -0.927   -17.910

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zfstensor (cm-1)
-1.226626  0.351038  -0.010994
 0.351038  0.283890  -0.091979
-0.010994 -0.091979  -0.662332

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.6133	-34.16367	6583.61034	-4.08204	6579.52830	6545.36463
2	C	3.3580	20.48733	-1758.48779	0.20734	-1758.28044	-1737.79311
3	C	-0.7863	60.03033	411.78010	-1.08265	410.69744	470.72778
4	C	1.1083	41.96133	-580.40221	0.65313	-579.74908	-537.78775
5	C	-1.0930	52.13567	572.37259	-0.74814	571.62444	623.76011
6	C	0.3997	23.93067	-209.29391	-1.25396	-210.54787	-186.61720
7	C	0.3693	52.84000	-193.40922	0.08840	-193.32082	-140.48082
8	C	-0.5187	53.38633	271.61078	-0.39285	271.21793	324.60427
9	C	-0.7683	47.45867	402.35401	0.38909	402.74311	450.20177
10	C	0.7150	44.07500	-374.42489	-0.86139	-375.28628	-331.21128
11	C	-1.2613	61.19100	660.52390	-1.28406	659.23985	720.43085
12	C	1.0957	68.94767	-573.76904	1.32339	-572.44566	-503.49799
13	C	0.7630	64.37033	-399.56110	-1.50870	-401.06980	-336.69947
14	C	1.0963	69.01633	-574.11816	1.16779	-572.95037	-503.93404
15	C	0.4303	176.50367	-225.35316	0.71586	-224.63730	-48.13363
16	H	0.4617	29.72233	-60.80395	0.32068	-60.48327	-30.76093
17	H	0.1177	29.94133	-15.49732	0.21293	-15.28440	14.65694
18	H	-0.0337	28.65500	4.43408	0.61585	5.04992	33.70492
19	C	0.4453	177.20133	-233.20823	-0.37967	-233.58790	-56.38657
20	H	-0.9853	29.96900	129.77363	-0.05113	129.72249	159.69149
21	H	-0.3997	28.74233	52.63822	-0.11969	52.51853	81.26086
22	H	-0.1073	29.36167	14.13637	-0.62980	13.50657	42.86824
23	C	0.4450	177.22367	-233.03367	-0.56047	-233.59414	-56.37048
24	C	0.4317	176.48400	-226.05139	0.71035	-225.34104	-48.85704
25	H	0.4660	29.70000	-61.37467	0.30163	-61.07304	-31.37304
26	H	-0.0323	28.63500	4.25847	0.57900	4.83748	33.47248
27	H	0.1177	29.91700	-15.49732	0.28310	-15.21422	14.70278
28	H	0.6053	23.79567	-79.72561	-0.27094	-79.99655	-56.20089
29	H	-0.9180	22.89533	120.90547	-0.36015	120.54532	143.44065
30	C	0.7610	64.32767	-398.51376	-1.74872	-400.26248	-335.93481
31	H	-0.1080	29.34667	14.22417	-0.71286	13.51132	42.85798
32	H	-0.4023	28.73233	52.98943	-0.30865	52.68079	81.41312
33	H	-0.9893	29.95000	130.30045	-0.11778	130.18267	160.13267
34	H	-1.1743	22.47733	154.66593	-0.13449	154.53144	177.00877
35	H	-0.3987	23.29667	52.50651	-0.19007	52.31645	75.61311
36	H	0.2100	23.44667	-27.65811	-0.07999	-27.73810	-4.29143
37	H	-0.2343	23.31300	30.86294	0.10492	30.96787	54.28087
38	Cr	33.4553	-3173.76433	77797.25132	-15.29040	77781.96093	74608.19659
39	Cl	1.4277	951.77500	-1916.87210	-14.66772	-1931.53982	-979.76482
40	Cl	1.4270	951.88800	-1915.97700	-13.16694	-1929.14393	-977.25593

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CrL2-STO-B3LYP-No-ZFS
Temperature: 298
Spin: 1.5

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atensor 1 N
-1.725 0.258 -0.274
0.258 -2.602 -0.094
-0.274 -0.094 -3.721
0.003 0.001 0.003
0.003 0.012 0.000

```

0.002 0.000 0.023

atensor 2 C
2.920 0.994 0.151
0.994 2.158 -0.004
0.151 -0.004 4.488
-0.040 -0.010 0.006
0.065 0.035 -0.010
0.002 0.000 0.005

atensor 3 C
0.226 0.215 -0.241
0.215 -0.342 -0.092
-0.241 -0.092 -1.537
0.004 -0.001 0.000
0.003 0.003 0.000
-0.001 0.000 0.001

atensor 4 C
0.497 0.088 0.270
0.088 -0.046 0.130
0.270 0.130 2.602
0.000 0.006 0.000
-0.005 -0.013 0.001
0.000 0.000 0.000

atensor 5 C
-0.352 -0.092 -0.145
-0.092 -0.885 -0.022
-0.145 -0.022 -1.502
0.002 -0.002 0.000
0.000 0.003 0.000
0.000 0.000 0.001

atensor 6 C
1.353 -0.481 -0.087
-0.481 -0.839 0.131
-0.087 0.131 0.481
0.013 -0.007 -0.001
-0.019 -0.023 0.004
-0.001 0.002 0.000

atensor 7 C
0.252 -0.102 0.054
-0.102 -0.041 0.048
0.054 0.048 0.621
0.001 0.001 0.000
-0.002 -0.005 0.001
0.000 0.000 0.000

atensor 8 C
-0.137 -0.161 -0.088
-0.161 -0.235 -0.014
-0.088 -0.014 -0.883
0.001 0.001 0.000
0.000 0.001 0.000
0.000 0.000 0.000

atensor 9 C
-1.014 -0.256 0.092
-0.256 -0.899 0.059
0.092 0.059 -0.412
-0.005 -0.009 0.001
0.000 0.001 0.000
0.001 0.001 0.000

atensor 10 C

1.391 -1.006 -0.188
-1.006 1.014 0.049
-0.188 0.049 -0.470
0.000 -0.004 0.001
-0.002 -0.008 0.001
0.000 0.001 0.003

atensor 11 C
0.014 -1.599 0.024
-1.599 -2.521 0.313
0.024 0.313 -0.475
0.052 0.009 0.002
-0.018 0.000 0.006
0.003 0.003 0.070

atensor 12 C
0.182 -0.669 0.099
-0.669 1.719 -2.270
0.099 -2.270 1.461
0.030 0.007 -0.014
-0.016 0.009 0.004
-0.001 0.023 0.058

atensor 13 C
1.749 1.651 -0.848
1.651 -0.147 -1.052
-0.848 -1.052 1.110
0.036 0.011 -0.008
-0.028 0.025 0.025
0.006 0.012 0.079

atensor 14 C
0.216 -0.077 0.202
-0.077 2.200 2.288
0.202 2.288 0.945
0.035 0.003 0.019
-0.015 0.007 0.005
0.009 -0.019 0.054

atensor 15 C
-0.136 -0.237 0.317
-0.237 0.303 -0.793
0.317 -0.793 0.941
0.003 0.001 -0.005
-0.002 0.002 0.000
0.000 0.007 0.002

atensor 16 H
-0.621 -0.221 0.249
-0.221 0.829 -1.428
0.249 -1.428 0.731
-0.007 0.002 -0.005
-0.004 0.002 -0.005
0.003 0.006 0.000

atensor 17 H
-0.211 -1.258 1.670
-1.258 -0.262 -1.749
1.670 -1.749 0.740
-0.007 -0.004 0.001
-0.007 -0.004 0.000
-0.003 0.011 -0.004

atensor 18 H
-1.964 -0.244 0.548
-0.244 -1.289 -1.798
0.548 -1.798 2.897

-0.013 -0.006 -0.007
-0.007 0.001 -0.009
0.005 0.014 -0.013

atensor 19 C
0.495 0.450 -0.613
0.450 0.100 -0.407
-0.613 -0.407 0.426
0.002 0.001 -0.002
-0.001 0.004 -0.002
0.001 0.005 0.006

atensor 20 H
-0.997 0.964 -0.834
0.964 -0.832 -0.897
-0.834 -0.898 -1.080
0.006 0.005 -0.010
0.003 0.003 -0.005
-0.001 0.003 0.002

atensor 21 H
-0.442 0.846 -2.224
0.845 -1.610 -1.135
-2.224 -1.135 1.115
0.003 -0.001 -0.017
0.005 0.004 -0.013
0.006 0.011 -0.004

atensor 22 H
1.497 1.219 -1.521
1.219 -1.177 -0.614
-1.521 -0.615 -0.848
0.013 -0.001 -0.008
0.008 0.004 -0.005
0.000 0.003 0.003

atensor 23 C
0.775 0.596 0.456
0.596 0.174 0.283
0.456 0.283 0.073
0.003 0.000 0.002
0.000 0.004 0.003
0.000 -0.005 0.006

atensor 24 C
-0.222 -0.040 -0.023
-0.040 0.479 0.884
-0.023 0.884 0.849
0.005 -0.001 0.005
-0.002 0.001 0.000
0.000 -0.007 0.002

atensor 25 H
-0.661 0.133 0.079
0.133 1.127 1.401
0.079 1.401 0.471
-0.006 0.001 0.007
-0.003 0.002 0.006
-0.001 -0.007 -0.001

atensor 26 H
-1.930 0.275 0.653
0.275 -0.868 2.198
0.653 2.198 2.441
-0.013 -0.009 0.008
-0.005 0.001 0.009
-0.005 -0.014 -0.013

atensor 27 H
-0.942 -0.913 -1.166
-0.913 0.146 2.132
-1.167 2.132 1.062
-0.007 -0.007 0.000
-0.007 -0.005 0.002
0.004 -0.009 -0.004

atensor 28 H
1.262 0.662 -0.213
0.662 0.406 -0.113
-0.213 -0.113 -0.101
0.006 0.002 0.000
0.006 0.005 -0.001
-0.001 0.000 0.004

atensor 29 H
0.254 0.274 -0.195
0.274 -1.600 -0.012
-0.195 -0.012 -1.133
0.004 0.000 0.000
0.001 -0.002 0.000
0.000 0.000 0.002

atensor 30 C
2.071 1.941 0.380
1.941 0.036 0.684
0.380 0.684 0.603
0.039 0.010 0.018
-0.032 0.022 -0.012
0.008 -0.009 0.079

atensor 31 H
2.053 1.448 0.610
1.448 -1.084 0.262
0.610 0.262 -1.499
0.014 -0.001 0.005
0.009 0.004 0.003
-0.004 -0.002 0.002

atensor 32 H
0.707 1.366 2.180
1.366 -1.374 1.053
2.180 1.053 -0.268
0.005 -0.002 0.015
0.008 0.004 0.010
-0.009 -0.011 -0.006

atensor 33 H
-0.627 1.227 0.576
1.227 -0.677 0.553
0.576 0.553 -1.604
0.008 0.005 0.007
0.005 0.003 0.003
-0.001 -0.004 0.000

atensor 34 H
-0.938 3.316 -0.517
3.316 1.376 -0.686
-0.517 -0.686 -3.514
0.029 0.045 -0.003
0.010 0.001 0.000
-0.001 -0.005 0.022

atensor 35 H
0.275 -0.239 -0.102

-0.239 -0.633 0.031
-0.102 0.031 -0.611
0.002 -0.002 0.000
0.000 -0.002 0.000
0.000 0.000 0.002

atensor 36 H
0.418 -0.334 -0.057
-0.334 0.167 0.025
-0.057 0.025 -0.156
0.000 -0.002 0.000
-0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.410 -0.693 -0.004
-0.693 0.567 0.021
-0.004 0.021 -0.725
-0.005 -0.003 0.001
-0.004 -0.001 0.001
0.001 0.000 0.002

atensor 38 Cr
21.322 2.896 -0.361
2.896 31.844 -1.009
-0.361 -1.009 19.789
0.867 -0.757 0.317
-0.913 1.076 0.220
0.325 0.200 2.981

atensor 39 Br
33.419 2.519 9.445
2.519 14.626 -25.998
9.445 -25.998 -21.269
-1.114 -0.236 -0.494
-0.331 -0.658 2.030
-0.602 1.301 1.764

atensor 40 Br
25.163 6.787 -22.677
6.787 19.563 20.831
-22.677 20.831 -17.925
-0.650 -0.433 1.200
-0.696 -0.970 -1.629
1.327 -0.946 1.610

orbtensor 1 N
-476.572 45.966 52.958
45.966 -549.869 20.779
52.958 20.779 -50.867
322.578 -4.686 -3.963
-4.686 332.592 -1.659
-3.963 -1.659 290.242

orbtensor 2 C
-293.409 30.147 25.156
30.147 -325.010 8.825
25.156 8.825 -87.398
259.459 5.935 -4.570
5.935 261.256 -2.605
-4.570 -2.605 226.874

orbtensor 3 C
-233.487 -40.863 25.742
-40.863 -283.310 17.527
25.742 17.527 -53.413
259.344 -1.569 -4.975

-1.569 254.757 -1.639
-4.975 -1.639 220.503

orbtensor 4 C
-310.853 -25.975 33.531
-25.975 -253.982 13.564
33.531 13.564 -64.316
252.906 2.524 -4.088
2.524 263.115 -2.487
-4.088 -2.487 222.619

orbtensor 5 C
-297.926 2.799 31.751
2.799 -277.827 11.719
31.751 11.719 -52.926
271.075 1.005 -5.340
1.005 261.475 -1.799
-5.340 -1.799 230.484

orbtensor 6 C
-291.965 14.824 22.897
14.824 -317.883 9.179
22.897 9.179 -110.483
269.758 0.329 -4.883
0.329 268.803 -1.994
-4.883 -1.994 232.427

orbtensor 7 C
-304.829 13.099 30.326
13.099 -223.878 6.820
30.326 6.820 -66.555
255.217 -5.534 -4.112
-5.534 260.549 -1.384
-4.112 -1.384 221.365

orbtensor 8 C
-265.278 48.474 24.635
48.474 -275.419 5.485
24.635 5.485 -56.149
259.487 2.297 -4.772
2.297 256.507 -2.050
-4.772 -2.050 223.812

orbtensor 9 C
-250.037 -33.555 26.114
-33.555 -299.309 16.875
26.114 16.875 -63.684
260.611 -6.818 -4.596
-6.818 256.025 -0.925
-4.596 -0.925 222.487

orbtensor 10 C
-308.192 -20.444 30.062
-20.444 -254.161 11.613
30.062 11.613 -86.129
267.493 1.538 -4.984
1.538 263.183 -1.986
-4.984 -1.986 229.886

orbtensor 11 C
-238.245 26.508 0.141
26.508 -121.352 -9.014
0.141 -9.014 -225.798
258.828 -2.525 -0.531
-2.525 231.658 1.480
-0.531 1.480 253.622

orbtensor 12 C
-221.584 21.039 -0.162
21.039 -104.721 23.284
-0.162 23.284 -248.539
261.953 -3.500 -4.917
-3.500 237.691 -1.735
-4.917 -1.735 256.059

orbtensor 13 C
-249.621 -4.265 10.897
-4.265 -93.402 11.528
10.897 11.528 -240.823
260.056 0.221 3.389
0.221 235.827 -0.625
3.389 -0.625 259.055

orbtensor 14 C
-223.546 12.285 -7.347
12.285 -111.564 -42.015
-7.347 -42.015 -239.642
264.043 -2.299 3.085
-2.299 238.325 4.227
3.085 4.227 253.330

orbtensor 15 C
-56.165 1.954 3.769
1.954 -46.033 2.407
3.769 2.407 -52.242
219.361 -1.744 4.727
-1.744 216.225 -3.245
4.727 -3.245 229.882

orbtensor 16 H
3.630 -0.775 -0.245
-0.775 2.470 1.612
-0.245 1.612 1.728
23.116 0.631 -0.091
0.631 29.397 -6.878
-0.091 -6.878 29.112

orbtensor 17 H
2.165 0.605 -2.689
0.605 3.292 2.148
-2.689 2.148 1.818
31.615 -0.678 1.062
-0.678 21.522 -1.934
1.062 -1.934 29.709

orbtensor 18 H
4.821 0.555 -0.602
0.555 3.883 1.392
-0.602 1.392 -2.831
21.931 -3.348 -0.314
-3.348 26.741 1.744
-0.314 1.744 31.314

orbtensor 19 C
-53.438 -0.963 -4.016
-0.963 -43.521 1.304
-4.016 1.304 -54.899
225.812 1.700 -8.224
1.700 216.202 0.090
-8.224 0.090 222.941

orbtensor 20 H
3.389 -0.917 1.378
-0.917 2.871 1.165

1.378	1.165	3.530
25.820	3.992	-4.250
3.992	29.044	-5.153
-4.250	-5.153	25.746

orbtensor 21 H

2.396	-1.309	3.303
-1.309	4.356	0.343
3.303	0.343	-1.146
25.816	2.990	-3.262
2.990	25.090	3.374
-3.262	3.374	29.919

orbtensor 22 H

-1.921	-0.949	1.989
-0.949	3.267	0.880
1.989	0.880	3.853
34.850	-1.563	-1.138
-1.563	22.671	-0.810
-1.138	-0.810	25.860

orbtensor 23 C

-51.531	-0.981	3.280
-0.981	-43.812	-2.276
3.280	-2.276	-56.424
229.583	2.461	6.274
2.461	216.191	-0.124
6.274	-0.124	219.188

orbtensor 24 C

-57.841	0.936	-2.403
0.936	-46.686	-3.232
-2.403	-3.232	-50.029
217.750	-1.018	-1.526
-1.018	217.099	5.055
-1.526	5.055	230.622

orbtensor 25 H

3.634	-1.157	-0.107
-1.157	2.102	-1.394
-0.107	-1.394	2.014
23.478	2.398	1.210
2.398	30.788	6.302
1.210	6.302	27.359

orbtensor 26 H

4.620	0.070	-1.317
0.070	3.463	-2.157
-1.317	-2.157	-2.266
22.769	-3.447	2.936
-3.447	26.522	-0.393
2.936	-0.393	30.694

orbtensor 27 H

3.425	0.272	2.277
0.272	2.755	-2.432
2.277	-2.432	1.015
30.983	-0.195	-1.405
-0.195	22.029	2.889
-1.405	2.889	29.835

orbtensor 28 H

-4.176	-6.263	0.666
-6.263	-16.041	1.560
0.666	1.560	-1.745
31.088	4.971	-1.427
4.971	40.867	-1.629

-1.427	-1.629	22.237
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orbtensor 29 H

-18.735	-3.868	2.289
-3.868	-2.991	0.517
2.289	0.517	-2.715
41.707	3.105	-2.748
3.105	30.357	-0.864
-2.748	-0.864	21.882

orbtensor 30 C

-254.129	-9.860	-6.262
-9.860	-97.315	-24.691
-6.262	-24.691	-232.467
258.330	0.332	-3.261
0.332	236.214	3.058
-3.261	3.058	260.398

orbtensor 31 H

-2.483	-1.242	-0.193
-1.242	3.062	-0.460
-0.193	-0.460	4.566
34.868	-1.270	-1.078
-1.270	22.915	1.469
-1.078	1.469	25.599

orbtensor 32 H

0.592	-1.803	-3.578
-1.803	4.274	-0.416
-3.578	-0.416	0.728
27.607	2.472	3.663
2.472	24.358	-3.577
3.663	-3.577	28.866

orbtensor 33 H

2.748	-1.278	-1.015
-1.278	2.623	-0.746
-1.015	-0.746	4.360
27.746	5.492	3.091
5.492	29.952	3.379
3.091	3.379	22.912

orbtensor 34 H

-7.387	6.439	0.515
6.439	-13.534	-0.152
0.515	-0.152	-0.702
34.767	-3.190	-1.794
-3.190	34.609	-0.390
-1.794	-0.390	19.680

orbtensor 35 H

-19.029	0.365	2.103
0.365	-2.628	-0.032
2.103	-0.032	-2.679
42.832	-0.523	-2.669
-0.523	30.081	-0.372
-2.669	-0.372	22.092

orbtensor 36 H

-7.844	8.317	0.227
8.317	-13.020	-0.522
0.227	-0.522	-2.670
34.046	-7.112	-1.112
-7.112	37.957	0.092
-1.112	0.092	22.555

orbtensor 37 H

```

-3.814   -5.721   0.669
-5.721  -17.019   1.579
0.669    1.579  -1.056
30.832   1.927  -1.348
1.927   40.682  -1.277
-1.348  -1.277   21.316

```

```

orbtensor 38 Cr
-5343.382  625.438 -128.318
625.438 -3555.510 -213.637
-128.318 -213.637 -6062.838
1802.652   0.265   0.146
0.265 1813.390 -0.532
0.146 -0.532 1803.912

```

```

orbtensor 39 Br
-555.392  -42.990   3.340
-42.990 -724.268  284.299
3.340  284.299 -606.505
3094.611  -1.243  -2.217
-1.243 3099.781   6.138
-2.217   6.138 3101.114

```

```

orbtensor 40 Br
-558.536 -111.412   0.058
-111.412 -781.331 -246.491
0.058 -246.491 -548.585
3096.169  -2.404   3.860
-2.404 3098.558  -5.472
3.860  -5.472 3100.777

```

```

gtensor (ppt)
-0.166   0.005   0.000
0.005  -0.151  -0.001
0.000  -0.001  -0.165
8.705   7.749  -2.155
7.749   7.818  -1.665
-2.155  -1.665  -4.601

```

```

averaging
2H Average:34
4H Average:29
9,10H Average:16,17,18,20,21,22
5H Average:35
8,11H Average:25,26,27,31,32,33
6H Average:36
3H Average:28
7H Average:37

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.6700	-43.96533	4903.67690	-5.83567	4897.84123	4853.87590
2	C	3.1887	13.92400	-1683.14790	0.11249	-1683.03541	-1669.11141
3	C	-0.5483	54.79800	289.43950	-1.54850	287.89100	342.68900
4	C	1.0133	36.49633	-534.89124	1.79169	-533.09955	-496.60322
5	C	-0.9110	44.78500	480.87427	-0.62102	480.25324	525.03824
6	C	0.3283	16.88567	-173.31180	0.76493	-172.54687	-155.66121
7	C	0.2760	47.28967	-145.68748	0.55197	-145.13551	-97.84585
8	C	-0.4177	47.65333	220.46669	-0.34802	220.11867	267.77200
9	C	-0.7763	42.03100	409.79003	0.82271	410.61275	452.64375
10	C	0.6433	37.36000	-339.58556	0.04818	-339.53738	-302.17738
11	C	-0.9533	52.90433	503.22005	2.80378	506.02384	558.92817
12	C	1.1530	60.28633	-608.61474	0.76229	-607.85245	-547.56612
13	C	0.9507	57.03067	-501.81244	-2.66093	-504.47338	-447.44271

14	C	1.1523	60.31533	-608.26284	0.76287	-607.49997	-547.18463
15	C	0.3717	170.34267	-196.18544	0.87281	-195.31263	-24.96996
16	H	0.3113	29.81767	-41.33171	0.12776	-41.20395	-11.38628
17	H	0.0840	30.04033	-11.15160	0.64738	-10.50422	19.53611
18	H	-0.1270	28.61967	16.86015	0.86709	17.72724	46.34691
19	C	0.3443	171.03233	-181.75745	-0.87856	-182.63602	-11.60368
20	H	-0.9660	30.13333	128.24336	-0.50722	127.73613	157.86947
21	H	-0.3113	28.81033	41.33171	-0.19284	41.13887	69.94921
22	H	-0.1693	29.52667	22.48020	-0.82603	21.65417	51.18084
23	C	0.3450	171.06500	-182.10935	-0.87866	-182.98802	-11.92302
24	C	0.3713	170.30500	-196.00949	0.87406	-195.13542	-24.83042
25	H	0.3107	29.79167	-41.24321	0.12808	-41.11513	-11.32346
26	H	-0.1273	28.60067	16.90440	0.86765	17.77205	46.37272
27	H	0.0833	30.01400	-11.06309	0.64761	-10.41548	19.59852
28	H	0.5273	24.07667	-70.00724	-0.44194	-70.44919	-46.37252
29	H	-0.8250	23.16833	109.52461	-0.21808	109.30653	132.47487
30	C	0.9500	57.01033	-501.46054	-2.66067	-504.12121	-447.11088
31	H	-0.1700	29.50900	22.56871	-0.82633	21.74237	51.25137
32	H	-0.3107	28.80833	41.24321	-0.19303	41.05018	69.85851
33	H	-0.9657	30.11367	128.19911	-0.50753	127.69158	157.80525
34	H	-1.0080	22.47767	133.81916	-1.92686	131.89230	154.36997
35	H	-0.3223	23.55633	42.79204	-0.01547	42.77657	66.33291
36	H	0.1430	23.67467	-18.98427	0.02417	-18.96010	4.71457
37	H	-0.1907	23.64700	25.31235	0.09788	25.41023	49.05723
38	Cr	25.9597	-3180.59200	60848.86728	27.71683	60876.58411	57695.99211
39	Br	8.9227	2469.78033	-4711.72609	-39.59141	-4751.31750	-2281.53717
40	Br	8.9303	2469.01733	-4715.77457	-39.58322	-4755.35778	-2286.34045

=====
 CrL2-STO-B3LYP-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 N
 -1.725 0.258 -0.274
 0.258 -2.602 -0.094
 -0.274 -0.094 -3.721
 0.003 0.001 0.003
 0.003 0.012 0.000
 0.002 0.000 0.023

atensor 2 C
 2.920 0.994 0.151
 0.994 2.158 -0.004
 0.151 -0.004 4.488
 -0.040 -0.010 0.006
 0.065 0.035 -0.010
 0.002 0.000 0.005

atensor 3 C
 0.226 0.215 -0.241
 0.215 -0.342 -0.092
 -0.241 -0.092 -1.537
 0.004 -0.001 0.000
 0.003 0.003 0.000
 -0.001 0.000 0.001

atensor 4 C
 0.497 0.088 0.270
 0.088 -0.046 0.130
 0.270 0.130 2.602
 0.000 0.006 0.000
 -0.005 -0.013 0.001
 0.000 0.000 0.000

atensor 5 C

-0.352 -0.092 -0.145
-0.092 -0.885 -0.022
-0.145 -0.022 -1.502
0.002 -0.002 0.000
0.000 0.003 0.000
0.000 0.000 0.001

atensor 6 C
1.353 -0.481 -0.087
-0.481 -0.839 0.131
-0.087 0.131 0.481
0.013 -0.007 -0.001
-0.019 -0.023 0.004
-0.001 0.002 0.000

atensor 7 C
0.252 -0.102 0.054
-0.102 -0.041 0.048
0.054 0.048 0.621
0.001 0.001 0.000
-0.002 -0.005 0.001
0.000 0.000 0.000

atensor 8 C
-0.137 -0.161 -0.088
-0.161 -0.235 -0.014
-0.088 -0.014 -0.883
0.001 0.001 0.000
0.000 0.001 0.000
0.000 0.000 0.000

atensor 9 C
-1.014 -0.256 0.092
-0.256 -0.899 0.059
0.092 0.059 -0.412
-0.005 -0.009 0.001
0.000 0.001 0.000
0.001 0.001 0.000

atensor 10 C
1.391 -1.006 -0.188
-1.006 1.014 0.049
-0.188 0.049 -0.470
0.000 -0.004 0.001
-0.002 -0.008 0.001
0.000 0.001 0.003

atensor 11 C
0.014 -1.599 0.024
-1.599 -2.521 0.313
0.024 0.313 -0.475
0.052 0.009 0.002
-0.018 0.000 0.006
0.003 0.003 0.070

atensor 12 C
0.182 -0.669 0.099
-0.669 1.719 -2.270
0.099 -2.270 1.461
0.030 0.007 -0.014
-0.016 0.009 0.004
-0.001 0.023 0.058

atensor 13 C
1.749 1.651 -0.848
1.651 -0.147 -1.052
-0.848 -1.052 1.110

0.036 0.011 -0.008
-0.028 0.025 0.025
0.006 0.012 0.079

atensor 14 C
0.216 -0.077 0.202
-0.077 2.200 2.288
0.202 2.288 0.945
0.035 0.003 0.019
-0.015 0.007 0.005
0.009 -0.019 0.054

atensor 15 C
-0.136 -0.237 0.317
-0.237 0.303 -0.793
0.317 -0.793 0.941
0.003 0.001 -0.005
-0.002 0.002 0.000
0.000 0.007 0.002

atensor 16 H
-0.621 -0.221 0.249
-0.221 0.829 -1.428
0.249 -1.428 0.731
-0.007 0.002 -0.005
-0.004 0.002 -0.005
0.003 0.006 0.000

atensor 17 H
-0.211 -1.258 1.670
-1.258 -0.262 -1.749
1.670 -1.749 0.740
-0.007 -0.004 0.001
-0.007 -0.004 0.000
-0.003 0.011 -0.004

atensor 18 H
-1.964 -0.244 0.548
-0.244 -1.289 -1.798
0.548 -1.798 2.897
-0.013 -0.006 -0.007
-0.007 0.001 -0.009
0.005 0.014 -0.013

atensor 19 C
0.495 0.450 -0.613
0.450 0.100 -0.407
-0.613 -0.407 0.426
0.002 0.001 -0.002
-0.001 0.004 -0.002
0.001 0.005 0.006

atensor 20 H
-0.997 0.964 -0.834
0.964 -0.832 -0.897
-0.834 -0.898 -1.080
0.006 0.005 -0.010
0.003 0.003 -0.005
-0.001 0.003 0.002

atensor 21 H
-0.442 0.846 -2.224
0.845 -1.610 -1.135
-2.224 -1.135 1.115
0.003 -0.001 -0.017
0.005 0.004 -0.013
0.006 0.011 -0.004

atensor 22 H
1.497 1.219 -1.521
1.219 -1.177 -0.614
-1.521 -0.615 -0.848
0.013 -0.001 -0.008
0.008 0.004 -0.005
0.000 0.003 0.003

atensor 23 C
0.775 0.596 0.456
0.596 0.174 0.283
0.456 0.283 0.073
0.003 0.000 0.002
0.000 0.004 0.003
0.000 -0.005 0.006

atensor 24 C
-0.222 -0.040 -0.023
-0.040 0.479 0.884
-0.023 0.884 0.849
0.005 -0.001 0.005
-0.002 0.001 0.000
0.000 -0.007 0.002

atensor 25 H
-0.661 0.133 0.079
0.133 1.127 1.401
0.079 1.401 0.471
-0.006 0.001 0.007
-0.003 0.002 0.006
-0.001 -0.007 -0.001

atensor 26 H
-1.930 0.275 0.653
0.275 -0.868 2.198
0.653 2.198 2.441
-0.013 -0.009 0.008
-0.005 0.001 0.009
-0.005 -0.014 -0.013

atensor 27 H
-0.942 -0.913 -1.166
-0.913 0.146 2.132
-1.167 2.132 1.062
-0.007 -0.007 0.000
-0.007 -0.005 0.002
0.004 -0.009 -0.004

atensor 28 H
1.262 0.662 -0.213
0.662 0.406 -0.113
-0.213 -0.113 -0.101
0.006 0.002 0.000
0.006 0.005 -0.001
-0.001 0.000 0.004

atensor 29 H
0.254 0.274 -0.195
0.274 -1.600 -0.012
-0.195 -0.012 -1.133
0.004 0.000 0.000
0.001 -0.002 0.000
0.000 0.000 0.002

atensor 30 C
2.071 1.941 0.380

1.941 0.036 0.684
0.380 0.684 0.603
0.039 0.010 0.018
-0.032 0.022 -0.012
0.008 -0.009 0.079

atensor 31 H
2.053 1.448 0.610
1.448 -1.084 0.262
0.610 0.262 -1.499
0.014 -0.001 0.005
0.009 0.004 0.003
-0.004 -0.002 0.002

atensor 32 H
0.707 1.366 2.180
1.366 -1.374 1.053
2.180 1.053 -0.268
0.005 -0.002 0.015
0.008 0.004 0.010
-0.009 -0.011 -0.006

atensor 33 H
-0.627 1.227 0.576
1.227 -0.677 0.553
0.576 0.553 -1.604
0.008 0.005 0.007
0.005 0.003 0.003
-0.001 -0.004 0.000

atensor 34 H
-0.938 3.316 -0.517
3.316 1.376 -0.686
-0.517 -0.686 -3.514
0.029 0.045 -0.003
0.010 0.001 0.000
-0.001 -0.005 0.022

atensor 35 H
0.275 -0.239 -0.102
-0.239 -0.633 0.031
-0.102 0.031 -0.611
0.002 -0.002 0.000
0.000 -0.002 0.000
0.000 0.000 0.002

atensor 36 H
0.418 -0.334 -0.057
-0.334 0.167 0.025
-0.057 0.025 -0.156
0.000 -0.002 0.000
-0.001 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.410 -0.693 -0.004
-0.693 0.567 0.021
-0.004 0.021 -0.725
-0.005 -0.003 0.001
-0.004 -0.001 0.001
0.001 0.000 0.002

atensor 38 Cr
21.322 2.896 -0.361
2.896 31.844 -1.009
-0.361 -1.009 19.789
0.867 -0.757 0.317

-0.913 1.076 0.220
0.325 0.200 2.981

atensor 39 Br
33.419 2.519 9.445
2.519 14.626 -25.998
9.445 -25.998 -21.269
-1.114 -0.236 -0.494
-0.331 -0.658 2.030
-0.602 1.301 1.764

atensor 40 Br
25.163 6.787 -22.677
6.787 19.563 20.831
-22.677 20.831 -17.925
-0.650 -0.433 1.200
-0.696 -0.970 -1.629
1.327 -0.946 1.610

orbtensor 1 N
-476.572 45.966 52.958
45.966 -549.869 20.779
52.958 20.779 -50.867
322.578 -4.686 -3.963
-4.686 332.592 -1.659
-3.963 -1.659 290.242

orbtensor 2 C
-293.409 30.147 25.156
30.147 -325.010 8.825
25.156 8.825 -87.398
259.459 5.935 -4.570
5.935 261.256 -2.605
-4.570 -2.605 226.874

orbtensor 3 C
-233.487 -40.863 25.742
-40.863 -283.310 17.527
25.742 17.527 -53.413
259.344 -1.569 -4.975
-1.569 254.757 -1.639
-4.975 -1.639 220.503

orbtensor 4 C
-310.853 -25.975 33.531
-25.975 -253.982 13.564
33.531 13.564 -64.316
252.906 2.524 -4.088
2.524 263.115 -2.487
-4.088 -2.487 222.619

orbtensor 5 C
-297.926 2.799 31.751
2.799 -277.827 11.719
31.751 11.719 -52.926
271.075 1.005 -5.340
1.005 261.475 -1.799
-5.340 -1.799 230.484

orbtensor 6 C
-291.965 14.824 22.897
14.824 -317.883 9.179
22.897 9.179 -110.483
269.758 0.329 -4.883
0.329 268.803 -1.994
-4.883 -1.994 232.427

orbtensor 7 C
-304.829 13.099 30.326
13.099 -223.878 6.820
30.326 6.820 -66.555
255.217 -5.534 -4.112
-5.534 260.549 -1.384
-4.112 -1.384 221.365

orbtensor 8 C
-265.278 48.474 24.635
48.474 -275.419 5.485
24.635 5.485 -56.149
259.487 2.297 -4.772
2.297 256.507 -2.050
-4.772 -2.050 223.812

orbtensor 9 C
-250.037 -33.555 26.114
-33.555 -299.309 16.875
26.114 16.875 -63.684
260.611 -6.818 -4.596
-6.818 256.025 -0.925
-4.596 -0.925 222.487

orbtensor 10 C
-308.192 -20.444 30.062
-20.444 -254.161 11.613
30.062 11.613 -86.129
267.493 1.538 -4.984
1.538 263.183 -1.986
-4.984 -1.986 229.886

orbtensor 11 C
-238.245 26.508 0.141
26.508 -121.352 -9.014
0.141 -9.014 -225.798
258.828 -2.525 -0.531
-2.525 231.658 1.480
-0.531 1.480 253.622

orbtensor 12 C
-221.584 21.039 -0.162
21.039 -104.721 23.284
-0.162 23.284 -248.539
261.953 -3.500 -4.917
-3.500 237.691 -1.735
-4.917 -1.735 256.059

orbtensor 13 C
-249.621 -4.265 10.897
-4.265 -93.402 11.528
10.897 11.528 -240.823
260.056 0.221 3.389
0.221 235.827 -0.625
3.389 -0.625 259.055

orbtensor 14 C
-223.546 12.285 -7.347
12.285 -111.564 -42.015
-7.347 -42.015 -239.642
264.043 -2.299 3.085
-2.299 238.325 4.227
3.085 4.227 253.330

orbtensor 15 C
-56.165 1.954 3.769
1.954 -46.033 2.407

3.769	2.407	-52.242
219.361	-1.744	4.727
-1.744	216.225	-3.245
4.727	-3.245	229.882

orbtensor 16 H

3.630	-0.775	-0.245
-0.775	2.470	1.612
-0.245	1.612	1.728
23.116	0.631	-0.091
0.631	29.397	-6.878
-0.091	-6.878	29.112

orbtensor 17 H

2.165	0.605	-2.689
0.605	3.292	2.148
-2.689	2.148	1.818
31.615	-0.678	1.062
-0.678	21.522	-1.934
1.062	-1.934	29.709

orbtensor 18 H

4.821	0.555	-0.602
0.555	3.883	1.392
-0.602	1.392	-2.831
21.931	-3.348	-0.314
-3.348	26.741	1.744
-0.314	1.744	31.314

orbtensor 19 C

-53.438	-0.963	-4.016
-0.963	-43.521	1.304
-4.016	1.304	-54.899
225.812	1.700	-8.224
1.700	216.202	0.090
-8.224	0.090	222.941

orbtensor 20 H

3.389	-0.917	1.378
-0.917	2.871	1.165
1.378	1.165	3.530
25.820	3.992	-4.250
3.992	29.044	-5.153
-4.250	-5.153	25.746

orbtensor 21 H

2.396	-1.309	3.303
-1.309	4.356	0.343
3.303	0.343	-1.146
25.816	2.990	-3.262
2.990	25.090	3.374
-3.262	3.374	29.919

orbtensor 22 H

-1.921	-0.949	1.989
-0.949	3.267	0.880
1.989	0.880	3.853
34.850	-1.563	-1.138
-1.563	22.671	-0.810
-1.138	-0.810	25.860

orbtensor 23 C

-51.531	-0.981	3.280
-0.981	-43.812	-2.276
3.280	-2.276	-56.424
229.583	2.461	6.274
2.461	216.191	-0.124

6.274 -0.124 219.188

orbtensor 24 C

-57.841 0.936 -2.403
0.936 -46.686 -3.232
-2.403 -3.232 -50.029
217.750 -1.018 -1.526
-1.018 217.099 5.055
-1.526 5.055 230.622

orbtensor 25 H

3.634 -1.157 -0.107
-1.157 2.102 -1.394
-0.107 -1.394 2.014
23.478 2.398 1.210
2.398 30.788 6.302
1.210 6.302 27.359

orbtensor 26 H

4.620 0.070 -1.317
0.070 3.463 -2.157
-1.317 -2.157 -2.266
22.769 -3.447 2.936
-3.447 26.522 -0.393
2.936 -0.393 30.694

orbtensor 27 H

3.425 0.272 2.277
0.272 2.755 -2.432
2.277 -2.432 1.015
30.983 -0.195 -1.405
-0.195 22.029 2.889
-1.405 2.889 29.835

orbtensor 28 H

-4.176 -6.263 0.666
-6.263 -16.041 1.560
0.666 1.560 -1.745
31.088 4.971 -1.427
4.971 40.867 -1.629
-1.427 -1.629 22.237

orbtensor 29 H

-18.735 -3.868 2.289
-3.868 -2.991 0.517
2.289 0.517 -2.715
41.707 3.105 -2.748
3.105 30.357 -0.864
-2.748 -0.864 21.882

orbtensor 30 C

-254.129 -9.860 -6.262
-9.860 -97.315 -24.691
-6.262 -24.691 -232.467
258.330 0.332 -3.261
0.332 236.214 3.058
-3.261 3.058 260.398

orbtensor 31 H

-2.483 -1.242 -0.193
-1.242 3.062 -0.460
-0.193 -0.460 4.566
34.868 -1.270 -1.078
-1.270 22.915 1.469
-1.078 1.469 25.599

orbtensor 32 H

0.592	-1.803	-3.578
-1.803	4.274	-0.416
-3.578	-0.416	0.728
27.607	2.472	3.663
2.472	24.358	-3.577
3.663	-3.577	28.866

orbtensor 33 H

2.748	-1.278	-1.015
-1.278	2.623	-0.746
-1.015	-0.746	4.360
27.746	5.492	3.091
5.492	29.952	3.379
3.091	3.379	22.912

orbtensor 34 H

-7.387	6.439	0.515
6.439	-13.534	-0.152
0.515	-0.152	-0.702
34.767	-3.190	-1.794
-3.190	34.609	-0.390
-1.794	-0.390	19.680

orbtensor 35 H

-19.029	0.365	2.103
0.365	-2.628	-0.032
2.103	-0.032	-2.679
42.832	-0.523	-2.669
-0.523	30.081	-0.372
-2.669	-0.372	22.092

orbtensor 36 H

-7.844	8.317	0.227
8.317	-13.020	-0.522
0.227	-0.522	-2.670
34.046	-7.112	-1.112
-7.112	37.957	0.092
-1.112	0.092	22.555

orbtensor 37 H

-3.814	-5.721	0.669
-5.721	-17.019	1.579
0.669	1.579	-1.056
30.832	1.927	-1.348
1.927	40.682	-1.277
-1.348	-1.277	21.316

orbtensor 38 Cr

-5343.382	625.438	-128.318
625.438	-3555.510	-213.637
-128.318	-213.637	-6062.838
1802.652	0.265	0.146
0.265	1813.390	-0.532
0.146	-0.532	1803.912

orbtensor 39 Br

-555.392	-42.990	3.340
-42.990	-724.268	284.299
3.340	284.299	-606.505
3094.611	-1.243	-2.217
-1.243	3099.781	6.138
-2.217	6.138	3101.114

orbtensor 40 Br

-558.536	-111.412	0.058
-111.412	-781.331	-246.491
0.058	-246.491	-548.585

3096.169 -2.404 3.860
 -2.404 3098.558 -5.472
 3.860 -5.472 3100.777

gtensor (ppt)
 -0.166 0.005 0.000
 0.005 -0.151 -0.001
 0.000 -0.001 -0.165
 8.705 7.749 -2.155
 7.749 7.818 -1.665
 -2.155 -1.665 -4.601

zfstensor (cm-1)
 -10.444475 -0.520473 0.539439
 -0.520473 -8.295005 0.173388
 0.539439 0.173388 -7.425240

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.6700	-43.96533	4903.81187	-18.35608	4885.45579	4841.49046
2	C	3.1887	13.92400	-1683.19423	1.01525	-1682.17898	-1668.25498
3	C	-0.5483	54.79800	289.44747	-4.65803	284.78944	339.58744
4	C	1.0133	36.49633	-534.90597	4.57505	-530.33092	-493.83459
5	C	-0.9110	44.78500	480.88750	-2.44127	478.44623	523.23123
6	C	0.3283	16.88567	-173.31657	-0.90084	-174.21741	-157.33175
7	C	0.2760	47.28967	-145.69149	1.09282	-144.59867	-97.30901
8	C	-0.4177	47.65333	220.47275	-1.30710	219.16566	266.81899
9	C	-0.7763	42.03100	409.80131	2.07877	411.88009	453.91109
10	C	0.6433	37.36000	-339.59491	-1.68274	-341.27765	-303.91765
11	C	-0.9533	52.90433	503.23390	2.90432	506.13822	559.04256
12	C	1.1530	60.28633	-608.63149	3.17312	-605.45837	-545.17204
13	C	0.9507	57.03067	-501.82625	-7.33955	-509.16580	-452.13514
14	C	1.1523	60.31533	-608.27958	3.74211	-604.53747	-544.22214
15	C	0.3717	170.34267	-196.19084	2.80519	-193.38565	-23.04298
16	H	0.3113	29.81767	-41.33285	0.74084	-40.59201	-10.77435
17	H	0.0840	30.04033	-11.15190	1.60499	-9.54691	20.49342
18	H	-0.1270	28.61967	16.86062	2.61538	19.47599	48.09566
19	C	0.3443	171.03233	-181.76245	-2.43639	-184.19885	-13.16652
20	H	-0.9660	30.13333	128.24689	-1.09090	127.15599	157.28932
21	H	-0.3113	28.81033	41.33285	-0.75304	40.57981	69.39015
22	H	-0.1693	29.52667	22.48082	-2.70910	19.77172	49.29839
23	C	0.3450	171.06500	-182.11437	-2.09866	-184.21303	-13.14803
24	C	0.3713	170.30500	-196.01488	2.92296	-193.09192	-22.78692
25	H	0.3107	29.79167	-41.24434	0.81549	-40.42885	-10.63718
26	H	-0.1273	28.60067	16.90487	2.74191	19.64678	48.24745
27	H	0.0833	30.01400	-11.06340	1.54879	-9.51461	20.49939
28	H	0.5273	24.07667	-70.00917	-1.23780	-71.24697	-47.17030
29	H	-0.8250	23.16833	109.52762	-1.01303	108.51459	131.68293
30	C	0.9500	57.01033	-501.47434	-6.83698	-508.31133	-451.30099
31	H	-0.1700	29.50900	22.56933	-2.55441	20.01492	49.52392
32	H	-0.3107	28.80833	41.24434	-0.42007	40.82428	69.63261
33	H	-0.9657	30.11367	128.20264	-0.96237	127.24027	157.35394
34	H	-1.0080	22.47767	133.82284	-3.63623	130.18661	152.66428
35	H	-0.3223	23.55633	42.79322	-0.37104	42.42218	65.97851
36	H	0.1430	23.67467	-18.98479	-0.11715	-19.10194	4.57273
37	H	-0.1907	23.64700	25.31305	0.29214	25.60519	49.25219
38	Cr	25.9597	-3180.59200	60850.54212	14.65976	60865.20187	57684.60987
39	Br	8.9227	2469.78033	-4711.85578	-117.26208	-4829.11786	-2359.33753
40	Br	8.9303	2469.01733	-4715.90437	-119.38547	-4835.28984	-2366.27250

CrL2-STO-BHLYP-No-ZFS

Temperature: 298

Spin: 1.5

atensor 1 N
-2.466 0.249 -0.327
0.249 -3.355 -0.114
-0.327 -0.114 -4.871
0.000 -0.008 0.004
0.003 0.022 0.000
0.004 0.001 0.028

atensor 2 C
3.367 0.997 0.133
0.997 2.538 -0.007
0.133 -0.007 4.803
-0.029 -0.005 0.005
0.046 0.013 -0.006
0.002 0.000 0.005

atensor 3 C
-0.328 0.214 -0.321
0.214 -0.865 -0.127
-0.321 -0.127 -2.703
0.002 -0.001 0.000
0.001 0.004 0.000
0.000 0.000 0.002

atensor 4 C
1.042 0.097 0.283
0.097 0.487 0.135
0.283 0.135 3.255
-0.003 0.003 0.000
0.000 -0.009 0.001
0.001 0.000 0.001

atensor 5 C
-0.733 -0.104 -0.226
-0.104 -1.283 -0.053
-0.226 -0.053 -2.512
0.001 -0.001 0.000
0.001 0.003 0.000
0.000 0.000 0.003

atensor 6 C
1.722 -0.496 -0.038
-0.496 -0.511 0.154
-0.038 0.154 1.217
0.007 -0.002 0.000
-0.017 -0.015 0.003
0.000 0.001 0.003

atensor 7 C
0.659 -0.100 0.134
-0.100 0.335 0.083
0.134 0.083 1.646
-0.001 0.001 0.000
-0.001 -0.004 0.000
0.000 0.000 0.001

atensor 8 C
-0.489 -0.156 -0.175
-0.156 -0.581 -0.050
-0.175 -0.050 -1.894
0.001 0.000 0.000
0.001 0.002 0.000
0.000 0.000 0.001

atensor 9 C
-0.654 -0.247 0.157

-0.247 -0.543 0.085
0.157 0.085 0.446
-0.005 -0.006 0.001
0.003 0.002 0.000
0.001 0.001 0.001

atensor 10 C
1.265 -1.051 -0.276
-1.051 0.908 0.017
-0.276 0.017 -1.293
-0.001 0.002 0.001
0.003 -0.006 0.000
0.001 0.000 0.006

atensor 11 C
-0.537 -1.657 0.023
-1.657 -3.182 0.325
0.023 0.325 -1.061
0.065 0.021 0.001
-0.029 -0.014 0.009
0.004 0.002 0.084

atensor 12 C
-0.204 -0.785 0.140
-0.785 0.991 -2.187
0.140 -2.187 1.146
0.054 0.005 -0.009
-0.008 0.005 0.029
0.002 0.036 0.072

atensor 13 C
1.432 1.669 -0.883
1.669 -0.683 -1.017
-0.883 -1.017 0.764
0.048 -0.002 -0.007
-0.034 0.021 0.026
0.007 0.024 0.087

atensor 14 C
-0.181 -0.207 0.197
-0.207 1.462 2.282
0.197 2.282 0.652
0.057 -0.002 0.013
-0.014 -0.001 -0.018
0.004 -0.029 0.075

atensor 15 C
-0.135 -0.242 0.318
-0.242 0.328 -0.803
0.318 -0.803 0.925
0.005 0.001 -0.006
-0.002 0.001 0.003
-0.002 0.009 0.000

atensor 16 H
-0.975 -0.233 0.241
-0.233 0.484 -1.449
0.241 -1.449 0.381
-0.003 0.003 -0.005
-0.003 0.000 0.001
0.002 0.012 -0.002

atensor 17 H
-0.292 -1.291 1.696
-1.291 -0.328 -1.786
1.696 -1.786 0.685
-0.005 0.002 -0.006

-0.003 -0.002 0.007
-0.011 0.018 -0.007

atensor 18 H
-2.067 -0.248 0.558
-0.248 -1.434 -1.838
0.558 -1.839 2.888
-0.005 -0.005 -0.009
-0.007 0.006 -0.002
0.001 0.022 -0.026

atensor 19 C
0.577 0.463 -0.618
0.463 0.193 -0.417
-0.618 -0.417 0.494
0.003 -0.001 0.001
-0.001 0.004 -0.001
0.004 0.006 0.006

atensor 20 H
-1.153 0.985 -0.838
0.985 -0.977 -0.922
-0.838 -0.922 -1.226
0.006 0.001 -0.005
0.000 0.004 -0.001
0.003 0.006 0.003

atensor 21 H
-0.478 0.851 -2.266
0.851 -1.711 -1.160
-2.266 -1.160 1.127
0.004 -0.004 -0.007
0.003 0.008 -0.009
0.017 0.016 -0.009

atensor 22 H
1.485 1.248 -1.553
1.248 -1.243 -0.630
-1.553 -0.630 -0.892
0.006 -0.006 -0.001
0.005 0.008 -0.003
0.008 0.005 0.007

atensor 23 C
0.858 0.611 0.455
0.611 0.268 0.287
0.455 0.287 0.139
0.002 -0.002 0.001
-0.001 0.004 0.002
-0.003 -0.005 0.007

atensor 24 C
-0.222 -0.043 -0.027
-0.043 0.507 0.890
-0.027 0.890 0.833
0.007 -0.001 0.005
-0.003 0.000 -0.003
0.001 -0.009 0.000

atensor 25 H
-1.011 0.128 0.086
0.128 0.786 1.424
0.086 1.424 0.112
-0.002 0.000 0.005
-0.004 -0.001 -0.001
-0.001 -0.012 -0.001

atensor 26 H
-2.032 0.284 0.666
0.284 -1.002 2.251
0.666 2.251 2.422
-0.004 -0.010 0.005
-0.008 0.003 0.000
-0.006 -0.024 -0.024

atensor 27 H
-1.033 -0.938 -1.181
-0.938 0.089 2.177
-1.181 2.177 1.009
-0.001 -0.002 0.004
-0.003 -0.005 -0.007
0.010 -0.019 -0.008

atensor 28 H
1.621 0.583 -0.222
0.583 0.586 -0.099
-0.222 -0.099 0.160
0.003 -0.001 0.000
0.003 0.004 0.000
0.000 0.000 0.006

atensor 29 H
0.083 0.296 -0.197
0.296 -1.813 -0.013
-0.197 -0.013 -1.314
0.000 -0.001 0.001
0.002 0.001 0.000
0.000 0.000 0.004

atensor 30 C
1.769 1.955 0.402
1.955 -0.505 0.665
0.402 0.665 0.248
0.051 -0.006 0.018
-0.039 0.017 -0.010
0.007 -0.015 0.087

atensor 31 H
2.053 1.482 0.626
1.482 -1.148 0.271
0.626 0.271 -1.558
0.005 -0.007 0.003
0.005 0.008 0.002
-0.008 -0.004 0.009

atensor 32 H
0.694 1.384 2.226
1.384 -1.469 1.086
2.226 1.086 -0.284
0.001 -0.008 0.006
0.003 0.008 0.007
-0.020 -0.016 -0.005

atensor 33 H
-0.781 1.254 0.579
1.254 -0.818 0.570
0.579 0.570 -1.756
0.006 0.000 0.005
0.000 0.003 0.001
-0.004 -0.007 0.003

atensor 34 H
-1.110 3.438 -0.534
3.438 1.311 -0.712

-0.534 -0.712 -3.767
0.024 0.017 0.000
-0.001 0.004 0.002
0.001 -0.001 0.033

atensor 35 H
0.107 -0.216 -0.113
-0.216 -1.019 0.036
-0.113 0.036 -0.854
-0.001 -0.001 0.000
0.002 -0.001 0.000
0.000 0.000 0.003

atensor 36 H
0.750 -0.225 -0.070
-0.225 0.441 0.011
-0.070 0.011 0.116
-0.001 0.000 0.000
0.001 -0.002 0.000
0.000 0.000 0.002

atensor 37 H
-0.739 -0.642 0.006
-0.642 0.376 0.012
0.006 0.012 -0.959
-0.003 0.001 0.001
0.000 -0.004 0.000
0.001 0.000 0.005

atensor 38 Cr
29.820 3.204 -0.453
3.204 40.301 -1.077
-0.453 -1.077 27.705
1.960 -0.778 0.307
-1.009 1.709 0.252
0.319 0.222 3.990

atensor 39 Br
30.114 2.902 8.017
2.902 12.276 -25.067
8.017 -25.067 -17.265
-0.563 -0.113 -0.263
-0.280 -0.641 1.234
-0.337 0.488 0.833

atensor 40 Br
22.999 7.240 -19.672
7.240 17.068 20.429
-19.672 20.429 -14.939
-0.319 -0.166 0.600
-0.507 -0.799 -0.971
0.700 -0.290 0.746

orbtensor 1 N
-480.395 41.301 56.268
41.301 -526.065 21.199
56.268 21.199 -30.964
321.624 -6.137 -3.697
-6.137 333.946 -1.517
-3.697 -1.517 290.730

orbtensor 2 C
-295.856 32.649 26.598
32.649 -329.993 9.291
26.598 9.291 -77.713
257.787 6.058 -4.497
6.058 261.330 -2.680

```

-4.497   -2.680   225.814

orbtensor 3 C
-228.203  -43.444   26.480
-43.444  -279.511   18.185
26.480   18.185  -43.523
257.531   -1.341   -5.165
-1.341   253.586   -1.775
-5.165   -1.775   217.326

orbtensor 4 C
-315.022  -30.421   35.355
-30.421  -255.133   14.628
35.355   14.628  -56.448
251.181    2.972   -4.118
2.972   262.644   -2.613
-4.118   -2.613   220.851

orbtensor 5 C
-296.212    3.051   32.592
3.051  -275.752   12.029
32.592   12.029  -44.609
272.293    1.208   -5.576
1.208   259.810   -1.766
-5.576   -1.766   229.967

orbtensor 6 C
-292.778   15.840   24.559
15.840  -323.219    9.997
24.559    9.997  -98.074
269.332    0.626   -4.802
0.626   269.505   -2.051
-4.802   -2.051   232.746

orbtensor 7 C
-306.866   16.277   31.464
16.277  -220.022    6.635
31.464    6.635  -58.721
254.106   -6.302   -4.137
-6.302   259.864   -1.335
-4.137   -1.335   219.744

orbtensor 8 C
-264.219   50.329   25.247
50.329  -271.414    5.368
25.247    5.368  -49.601
258.912    2.838   -4.839
2.838   256.132   -2.145
-4.839   -2.145   222.953

orbtensor 9 C
-249.521  -36.434   27.349
-36.434  -298.691   17.679
27.349   17.679  -54.767
259.275   -6.909   -4.765
-6.909   254.606   -0.980
-4.765   -0.980   219.818

orbtensor 10 C
-308.608  -24.248   31.504
-24.248  -246.467   12.175
31.504   12.175  -77.262
268.190    2.595   -5.299
2.595   261.606   -2.108
-5.299   -2.108   228.604

orbtensor 11 C

```

```
-233.443  29.785  0.930
29.785 -111.557 -9.312
0.930  -9.312 -213.468
258.331  -1.859  -0.353
-1.859  229.978  1.545
-0.353  1.545  254.769
```

```
orbtensor 12 C
-213.932  22.214  -0.200
22.214  -97.776  27.051
-0.200  27.051 -239.087
264.143  -3.246  -5.839
-3.246  238.244  -1.314
-5.839  -1.314  255.621
```

```
orbtensor 13 C
-247.680  -5.618  11.450
-5.618  -84.461  13.441
11.450  13.441 -235.406
260.811  -0.037  4.956
-0.037  235.679  -0.466
4.956  -0.466  259.257
```

```
orbtensor 14 C
-215.738  12.567  -6.841
12.567 -105.361 -45.621
-6.841  -45.621 -229.543
266.512  -2.116  3.241
-2.116  238.771  3.637
3.241  3.637  252.719
```

```
orbtensor 15 C
-44.664  1.817  2.116
1.817 -36.203  3.558
2.116  3.558 -44.021
215.326  -1.801  5.196
-1.801  212.244  -3.799
5.196  -3.799  226.968
```

```
orbtensor 16 H
3.846  -0.639  -0.374
-0.639  3.107  1.353
-0.374  1.353  2.119
22.899  0.612  -0.053
0.612  28.916  -6.657
-0.053  -6.657  28.767
```

```
orbtensor 17 H
3.234  0.715  -2.967
0.715  3.214  2.493
-2.967  2.493  1.981
30.898  -0.740  0.991
-0.740  21.348  -2.011
0.991  -2.011  29.534
```

```
orbtensor 18 H
5.371  0.223  -0.881
0.223  4.557  2.175
-0.881  2.175  -2.743
21.568  -3.250  -0.247
-3.250  26.312  1.379
-0.247  1.379  30.927
```

```
orbtensor 19 C
-43.684  -1.423  -2.320
-1.423  -33.925  1.735
-2.320  1.735  -45.747
```

222.449	1.812	-8.791
1.812	212.262	-0.073
-8.791	-0.073	219.803

orbtensor 20 H

3.707	-0.808	1.280
-0.808	3.626	0.929
1.280	0.929	3.808
25.565	3.883	-4.170
3.883	28.542	-4.969
-4.170	-4.969	25.469

orbtensor 21 H

2.834	-1.361	3.666
-1.361	4.914	0.906
3.666	0.906	-0.637
25.531	3.006	-3.363
3.006	24.723	3.094
-3.363	3.094	29.405

orbtensor 22 H

-1.209	-1.401	2.389
-1.401	3.348	0.926
2.389	0.926	4.171
34.379	-1.345	-1.284
-1.345	22.526	-0.817
-1.284	-0.817	25.680

orbtensor 23 C

-42.629	-1.708	1.716
-1.708	-34.307	-2.537
1.716	-2.537	-46.352
226.510	2.679	6.804
2.679	212.297	0.062
6.804	0.062	215.731

orbtensor 24 C

-45.725	0.605	-1.703
0.605	-37.122	-4.505
-1.703	-4.505	-42.162
213.556	-0.952	-1.678
-0.952	213.246	5.717
-1.678	5.717	227.740

orbtensor 25 H

3.916	-0.953	0.028
-0.953	2.781	-1.204
0.028	-1.204	2.288
23.237	2.321	1.156
2.321	30.264	6.113
1.156	6.113	27.082

orbtensor 26 H

5.291	-0.431	-1.124
-0.431	3.969	-2.889
-1.124	-2.889	-2.138
22.366	-3.268	2.848
-3.268	26.165	-0.066
2.848	-0.066	30.274

orbtensor 27 H

4.567	0.311	2.303
0.311	2.600	-2.767
2.303	-2.767	1.172
30.336	-0.221	-1.209
-0.221	21.872	2.971
-1.209	2.971	29.573

orbtensor 28 H
-4.280 -6.107 0.631
-6.107 -15.740 1.510
0.631 1.510 -2.027
31.103 4.858 -1.422
4.858 40.868 -1.614
-1.422 -1.614 22.245

orbtensor 29 H
-18.667 -3.975 2.212
-3.975 -3.031 0.499
2.212 0.499 -3.280
41.473 3.107 -2.712
3.107 30.358 -0.861
-2.712 -0.861 21.927

orbtensor 30 C
-252.190 -11.694 -5.699
-11.694 -88.780 -26.521
-5.699 -26.521 -226.647
258.297 -0.110 -4.724
-0.110 236.050 3.070
-4.724 3.070 261.406

orbtensor 31 H
-1.978 -1.723 -0.589
-1.723 3.149 -0.345
-0.589 -0.345 5.085
34.481 -1.041 -0.904
-1.041 22.765 1.412
-0.904 1.412 25.340

orbtensor 32 H
0.859 -2.033 -3.849
-2.033 4.715 -0.929
-3.849 -0.929 1.518
27.354 2.562 3.684
2.562 24.048 -3.334
3.684 -3.334 28.265

orbtensor 33 H
3.103 -1.110 -0.957
-1.110 3.408 -0.594
-0.957 -0.594 4.554
27.456 5.336 3.034
5.336 29.419 3.259
3.034 3.259 22.705

orbtensor 34 H
-7.009 6.455 0.512
6.455 -13.100 -0.157
0.512 -0.157 -0.338
34.513 -3.379 -1.761
-3.379 34.328 -0.355
-1.761 -0.355 19.600

orbtensor 35 H
-18.925 0.567 2.003
0.567 -2.825 -0.075
2.003 -0.075 -3.258
42.784 -0.638 -2.628
-0.638 30.271 -0.356
-2.628 -0.356 22.308

orbtensor 36 H
-7.772 8.044 0.188

8.044 -12.875 -0.513
 0.188 -0.513 -3.004
 33.940 -6.969 -1.097
 -6.969 38.039 0.074
 -1.097 0.074 22.628

orbtensor 37 H
 -3.703 -5.788 0.639
 -5.788 -16.642 1.558
 0.639 1.558 -1.178
 30.608 1.977 -1.359
 1.977 40.347 -1.281
 -1.359 -1.281 21.028

orbtensor 38 Cr
 -5899.042 837.148 -189.852
 837.148 -3990.001 -268.001
 -189.852 -268.001 -7002.128
 1801.320 0.524 0.155
 0.524 1811.911 -0.548
 0.155 -0.548 1802.755

orbtensor 39 Br
 -161.295 -18.906 29.967
 -18.906 -386.159 65.196
 29.967 65.196 -288.264
 3095.416 -1.278 -2.164
 -1.278 3100.251 5.955
 -2.164 5.955 3101.720

orbtensor 40 Br
 -184.091 -37.644 -52.315
 -37.644 -398.844 -45.724
 -52.315 -45.724 -254.864
 3096.936 -2.398 3.762
 -2.398 3099.069 -5.273
 3.762 -5.273 3101.381

gtensor (ppt)
 -0.173 0.005 0.000
 0.005 -0.156 -0.002
 0.000 -0.002 -0.172
 -0.301 7.721 -2.392
 7.721 -0.456 -1.799
 -2.392 -1.799 -15.438

averaging
 2H Average:34
 4H Average:29
 9,10H Average:16,17,18,20,21,22
 5H Average:35
 8,11H Average:25,26,27,31,32,33
 6H Average:36
 3H Average:28
 7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.5473	-30.37467	6484.51500	-7.73420	6476.78080	6446.40613
2	C	3.5657	13.78967	-1873.34952	0.31211	-1873.03741	-1859.24775
3	C	-1.2960	59.06867	680.89959	-2.32474	678.57485	737.64352
4	C	1.5910	36.02433	-835.88831	2.22513	-833.66318	-797.63885
5	C	-1.5070	48.49900	791.75593	-1.29806	790.45787	838.95687
6	C	0.8077	19.17067	-424.33635	1.24966	-423.08669	-403.91602

7	C	0.8787	49.36833	-461.63871	1.23132	-460.40739	-411.03906
8	C	-0.9867	50.92100	518.38035	-1.07673	517.30362	568.22462
9	C	-0.2510	43.57333	131.87176	1.35319	133.22494	176.79828
10	C	0.2930	42.02100	-153.93795	-0.77917	-154.71711	-112.69611
11	C	-1.5483	61.53667	813.47186	3.10469	816.57655	878.11322
12	C	0.6880	69.07100	-361.46522	1.14984	-360.31537	-291.24437
13	C	0.5563	62.73333	-292.28946	-2.54496	-294.83442	-232.10109
14	C	0.6880	69.12000	-361.46522	1.15224	-360.31298	-291.19298
15	C	0.3747	176.55000	-196.84443	0.93864	-195.90579	-19.35579
16	H	-0.0383	29.88467	5.06523	0.13101	5.19624	35.08090
17	H	0.0170	30.06967	-2.24632	0.69701	-1.54931	28.52036
18	H	-0.2127	28.66400	28.10102	1.02262	29.12364	57.78764
19	C	0.4257	177.05267	-223.63909	-0.91942	-224.55850	-47.50584
20	H	-1.1143	30.23900	147.24406	-0.53335	146.71071	176.94971
21	H	-0.3530	28.92333	46.64417	-0.13336	46.51082	75.43415
22	H	-0.2097	29.63167	27.70461	-0.86730	26.83731	56.46898
23	C	0.4260	177.08333	-223.81422	-0.91890	-224.73312	-47.64979
24	C	0.3750	176.51100	-197.01956	0.93979	-196.07976	-19.56876
25	H	-0.0390	29.85600	5.15332	0.13156	5.28488	35.14088
26	H	-0.2123	28.64233	28.05698	1.02353	29.08051	57.72284
27	H	0.0170	30.04000	-2.24632	0.69736	-1.54896	28.49104
28	H	0.7933	24.05633	-104.82826	-0.44042	-105.26868	-81.21235
29	H	-1.0130	22.92667	133.85424	-0.22442	133.62981	156.55648
30	C	0.5557	62.71200	-291.93920	-2.54452	-294.48372	-231.77172
31	H	-0.2103	29.61400	27.79270	-0.86733	26.92537	56.53937
32	H	-0.3517	28.91967	46.46799	-0.13324	46.33475	75.25442
33	H	-1.1143	30.21500	147.24406	-0.53355	146.71052	176.92552
34	H	-1.1683	22.66467	154.37943	-2.13646	152.24298	174.90764
35	H	-0.5883	23.45167	77.74029	-0.02462	77.71566	101.16733
36	H	0.4353	23.65200	-57.52341	-0.03593	-57.55934	-33.90734
37	H	-0.4413	23.48667	58.31623	0.05165	58.36788	81.85455
38	Cr	35.1617	-3825.06167	82032.84095	35.41192	82068.25288	78243.19121
39	Br	8.2513	2820.55633	-4336.85010	-40.81880	-4377.66891	-1557.11257
40	Br	8.2520	2819.86233	-4337.20050	-40.79808	-4377.99858	-1558.13625

=====
CrL2-STO-BHLYP-ORCA

Temperature: 298

Spin: 1.5

atensor 1 N

-2.466 0.249 -0.327
0.249 -3.355 -0.114
-0.327 -0.114 -4.871
0.000 -0.008 0.004
0.003 0.022 0.000
0.004 0.001 0.028

atensor 2 C

3.367 0.997 0.133
0.997 2.538 -0.007
0.133 -0.007 4.803
-0.029 -0.005 0.005
0.046 0.013 -0.006
0.002 0.000 0.005

atensor 3 C

-0.328 0.214 -0.321
0.214 -0.865 -0.127
-0.321 -0.127 -2.703
0.002 -0.001 0.000
0.001 0.004 0.000
0.000 0.000 0.002

atensor 4 C

1.042 0.097 0.283

0.097 0.487 0.135
0.283 0.135 3.255
-0.003 0.003 0.000
0.000 -0.009 0.001
0.001 0.000 0.001

atensor 5 C
-0.733 -0.104 -0.226
-0.104 -1.283 -0.053
-0.226 -0.053 -2.512
0.001 -0.001 0.000
0.001 0.003 0.000
0.000 0.000 0.003

atensor 6 C
1.722 -0.496 -0.038
-0.496 -0.511 0.154
-0.038 0.154 1.217
0.007 -0.002 0.000
-0.017 -0.015 0.003
0.000 0.001 0.003

atensor 7 C
0.659 -0.100 0.134
-0.100 0.335 0.083
0.134 0.083 1.646
-0.001 0.001 0.000
-0.001 -0.004 0.000
0.000 0.000 0.001

atensor 8 C
-0.489 -0.156 -0.175
-0.156 -0.581 -0.050
-0.175 -0.050 -1.894
0.001 0.000 0.000
0.001 0.002 0.000
0.000 0.000 0.001

atensor 9 C
-0.654 -0.247 0.157
-0.247 -0.543 0.085
0.157 0.085 0.446
-0.005 -0.006 0.001
0.003 0.002 0.000
0.001 0.001 0.001

atensor 10 C
1.265 -1.051 -0.276
-1.051 0.908 0.017
-0.276 0.017 -1.293
-0.001 0.002 0.001
0.003 -0.006 0.000
0.001 0.000 0.006

atensor 11 C
-0.537 -1.657 0.023
-1.657 -3.182 0.325
0.023 0.325 -1.061
0.065 0.021 0.001
-0.029 -0.014 0.009
0.004 0.002 0.084

atensor 12 C
-0.204 -0.785 0.140
-0.785 0.991 -2.187
0.140 -2.187 1.146
0.054 0.005 -0.009

-0.008 0.005 0.029
0.002 0.036 0.072

atensor 13 C
1.432 1.669 -0.883
1.669 -0.683 -1.017
-0.883 -1.017 0.764
0.048 -0.002 -0.007
-0.034 0.021 0.026
0.007 0.024 0.087

atensor 14 C
-0.181 -0.207 0.197
-0.207 1.462 2.282
0.197 2.282 0.652
0.057 -0.002 0.013
-0.014 -0.001 -0.018
0.004 -0.029 0.075

atensor 15 C
-0.135 -0.242 0.318
-0.242 0.328 -0.803
0.318 -0.803 0.925
0.005 0.001 -0.006
-0.002 0.001 0.003
-0.002 0.009 0.000

atensor 16 H
-0.975 -0.233 0.241
-0.233 0.484 -1.449
0.241 -1.449 0.381
-0.003 0.003 -0.005
-0.003 0.000 0.001
0.002 0.012 -0.002

atensor 17 H
-0.292 -1.291 1.696
-1.291 -0.328 -1.786
1.696 -1.786 0.685
-0.005 0.002 -0.006
-0.003 -0.002 0.007
-0.011 0.018 -0.007

atensor 18 H
-2.067 -0.248 0.558
-0.248 -1.434 -1.838
0.558 -1.839 2.888
-0.005 -0.005 -0.009
-0.007 0.006 -0.002
0.001 0.022 -0.026

atensor 19 C
0.577 0.463 -0.618
0.463 0.193 -0.417
-0.618 -0.417 0.494
0.003 -0.001 0.001
-0.001 0.004 -0.001
0.004 0.006 0.006

atensor 20 H
-1.153 0.985 -0.838
0.985 -0.977 -0.922
-0.838 -0.922 -1.226
0.006 0.001 -0.005
0.000 0.004 -0.001
0.003 0.006 0.003

atensor 21 H
-0.478 0.851 -2.266
0.851 -1.711 -1.160
-2.266 -1.160 1.127
0.004 -0.004 -0.007
0.003 0.008 -0.009
0.017 0.016 -0.009

atensor 22 H
1.485 1.248 -1.553
1.248 -1.243 -0.630
-1.553 -0.630 -0.892
0.006 -0.006 -0.001
0.005 0.008 -0.003
0.008 0.005 0.007

atensor 23 C
0.858 0.611 0.455
0.611 0.268 0.287
0.455 0.287 0.139
0.002 -0.002 0.001
-0.001 0.004 0.002
-0.003 -0.005 0.007

atensor 24 C
-0.222 -0.043 -0.027
-0.043 0.507 0.890
-0.027 0.890 0.833
0.007 -0.001 0.005
-0.003 0.000 -0.003
0.001 -0.009 0.000

atensor 25 H
-1.011 0.128 0.086
0.128 0.786 1.424
0.086 1.424 0.112
-0.002 0.000 0.005
-0.004 -0.001 -0.001
-0.001 -0.012 -0.001

atensor 26 H
-2.032 0.284 0.666
0.284 -1.002 2.251
0.666 2.251 2.422
-0.004 -0.010 0.005
-0.008 0.003 0.000
-0.006 -0.024 -0.024

atensor 27 H
-1.033 -0.938 -1.181
-0.938 0.089 2.177
-1.181 2.177 1.009
-0.001 -0.002 0.004
-0.003 -0.005 -0.007
0.010 -0.019 -0.008

atensor 28 H
1.621 0.583 -0.222
0.583 0.586 -0.099
-0.222 -0.099 0.160
0.003 -0.001 0.000
0.003 0.004 0.000
0.000 0.000 0.006

atensor 29 H
0.083 0.296 -0.197
0.296 -1.813 -0.013

-0.197 -0.013 -1.314
0.000 -0.001 0.001
0.002 0.001 0.000
0.000 0.000 0.004

atensor 30 C
1.769 1.955 0.402
1.955 -0.505 0.665
0.402 0.665 0.248
0.051 -0.006 0.018
-0.039 0.017 -0.010
0.007 -0.015 0.087

atensor 31 H
2.053 1.482 0.626
1.482 -1.148 0.271
0.626 0.271 -1.558
0.005 -0.007 0.003
0.005 0.008 0.002
-0.008 -0.004 0.009

atensor 32 H
0.694 1.384 2.226
1.384 -1.469 1.086
2.226 1.086 -0.284
0.001 -0.008 0.006
0.003 0.008 0.007
-0.020 -0.016 -0.005

atensor 33 H
-0.781 1.254 0.579
1.254 -0.818 0.570
0.579 0.570 -1.756
0.006 0.000 0.005
0.000 0.003 0.001
-0.004 -0.007 0.003

atensor 34 H
-1.110 3.438 -0.534
3.438 1.311 -0.712
-0.534 -0.712 -3.767
0.024 0.017 0.000
-0.001 0.004 0.002
0.001 -0.001 0.033

atensor 35 H
0.107 -0.216 -0.113
-0.216 -1.019 0.036
-0.113 0.036 -0.854
-0.001 -0.001 0.000
0.002 -0.001 0.000
0.000 0.000 0.003

atensor 36 H
0.750 -0.225 -0.070
-0.225 0.441 0.011
-0.070 0.011 0.116
-0.001 0.000 0.000
0.001 -0.002 0.000
0.000 0.000 0.002

atensor 37 H
-0.739 -0.642 0.006
-0.642 0.376 0.012
0.006 0.012 -0.959
-0.003 0.001 0.001
0.000 -0.004 0.000

0.001 0.000 0.005

atensor 38 Cr

29.820 3.204 -0.453
3.204 40.301 -1.077
-0.453 -1.077 27.705
1.960 -0.778 0.307
-1.009 1.709 0.252
0.319 0.222 3.990

atensor 39 Br

30.114 2.902 8.017
2.902 12.276 -25.067
8.017 -25.067 -17.265
-0.563 -0.113 -0.263
-0.280 -0.641 1.234
-0.337 0.488 0.833

atensor 40 Br

22.999 7.240 -19.672
7.240 17.068 20.429
-19.672 20.429 -14.939
-0.319 -0.166 0.600
-0.507 -0.799 -0.971
0.700 -0.290 0.746

orbtensor 1 N

-480.395 41.301 56.268
41.301 -526.065 21.199
56.268 21.199 -30.964
321.624 -6.137 -3.697
-6.137 333.946 -1.517
-3.697 -1.517 290.730

orbtensor 2 C

-295.856 32.649 26.598
32.649 -329.993 9.291
26.598 9.291 -77.713
257.787 6.058 -4.497
6.058 261.330 -2.680
-4.497 -2.680 225.814

orbtensor 3 C

-228.203 -43.444 26.480
-43.444 -279.511 18.185
26.480 18.185 -43.523
257.531 -1.341 -5.165
-1.341 253.586 -1.775
-5.165 -1.775 217.326

orbtensor 4 C

-315.022 -30.421 35.355
-30.421 -255.133 14.628
35.355 14.628 -56.448
251.181 2.972 -4.118
2.972 262.644 -2.613
-4.118 -2.613 220.851

orbtensor 5 C

-296.212 3.051 32.592
3.051 -275.752 12.029
32.592 12.029 -44.609
272.293 1.208 -5.576
1.208 259.810 -1.766
-5.576 -1.766 229.967

orbtensor 6 C

-292.778	15.840	24.559
15.840	-323.219	9.997
24.559	9.997	-98.074
269.332	0.626	-4.802
0.626	269.505	-2.051
-4.802	-2.051	232.746

orbtensor 7 C

-306.866	16.277	31.464
16.277	-220.022	6.635
31.464	6.635	-58.721
254.106	-6.302	-4.137
-6.302	259.864	-1.335
-4.137	-1.335	219.744

orbtensor 8 C

-264.219	50.329	25.247
50.329	-271.414	5.368
25.247	5.368	-49.601
258.912	2.838	-4.839
2.838	256.132	-2.145
-4.839	-2.145	222.953

orbtensor 9 C

-249.521	-36.434	27.349
-36.434	-298.691	17.679
27.349	17.679	-54.767
259.275	-6.909	-4.765
-6.909	254.606	-0.980
-4.765	-0.980	219.818

orbtensor 10 C

-308.608	-24.248	31.504
-24.248	-246.467	12.175
31.504	12.175	-77.262
268.190	2.595	-5.299
2.595	261.606	-2.108
-5.299	-2.108	228.604

orbtensor 11 C

-233.443	29.785	0.930
29.785	-111.557	-9.312
0.930	-9.312	-213.468
258.331	-1.859	-0.353
-1.859	229.978	1.545
-0.353	1.545	254.769

orbtensor 12 C

-213.932	22.214	-0.200
22.214	-97.776	27.051
-0.200	27.051	-239.087
264.143	-3.246	-5.839
-3.246	238.244	-1.314
-5.839	-1.314	255.621

orbtensor 13 C

-247.680	-5.618	11.450
-5.618	-84.461	13.441
11.450	13.441	-235.406
260.811	-0.037	4.956
-0.037	235.679	-0.466
4.956	-0.466	259.257

orbtensor 14 C

-215.738	12.567	-6.841
12.567	-105.361	-45.621
-6.841	-45.621	-229.543

266.512	-2.116	3.241
-2.116	238.771	3.637
3.241	3.637	252.719

orbtensor 15 C

-44.664	1.817	2.116
1.817	-36.203	3.558
2.116	3.558	-44.021
215.326	-1.801	5.196
-1.801	212.244	-3.799
5.196	-3.799	226.968

orbtensor 16 H

3.846	-0.639	-0.374
-0.639	3.107	1.353
-0.374	1.353	2.119
22.899	0.612	-0.053
0.612	28.916	-6.657
-0.053	-6.657	28.767

orbtensor 17 H

3.234	0.715	-2.967
0.715	3.214	2.493
-2.967	2.493	1.981
30.898	-0.740	0.991
-0.740	21.348	-2.011
0.991	-2.011	29.534

orbtensor 18 H

5.371	0.223	-0.881
0.223	4.557	2.175
-0.881	2.175	-2.743
21.568	-3.250	-0.247
-3.250	26.312	1.379
-0.247	1.379	30.927

orbtensor 19 C

-43.684	-1.423	-2.320
-1.423	-33.925	1.735
-2.320	1.735	-45.747
222.449	1.812	-8.791
1.812	212.262	-0.073
-8.791	-0.073	219.803

orbtensor 20 H

3.707	-0.808	1.280
-0.808	3.626	0.929
1.280	0.929	3.808
25.565	3.883	-4.170
3.883	28.542	-4.969
-4.170	-4.969	25.469

orbtensor 21 H

2.834	-1.361	3.666
-1.361	4.914	0.906
3.666	0.906	-0.637
25.531	3.006	-3.363
3.006	24.723	3.094
-3.363	3.094	29.405

orbtensor 22 H

-1.209	-1.401	2.389
-1.401	3.348	0.926
2.389	0.926	4.171
34.379	-1.345	-1.284
-1.345	22.526	-0.817
-1.284	-0.817	25.680

orbtensor 23 C
-42.629 -1.708 1.716
-1.708 -34.307 -2.537
1.716 -2.537 -46.352
226.510 2.679 6.804
2.679 212.297 0.062
6.804 0.062 215.731

orbtensor 24 C
-45.725 0.605 -1.703
0.605 -37.122 -4.505
-1.703 -4.505 -42.162
213.556 -0.952 -1.678
-0.952 213.246 5.717
-1.678 5.717 227.740

orbtensor 25 H
3.916 -0.953 0.028
-0.953 2.781 -1.204
0.028 -1.204 2.288
23.237 2.321 1.156
2.321 30.264 6.113
1.156 6.113 27.082

orbtensor 26 H
5.291 -0.431 -1.124
-0.431 3.969 -2.889
-1.124 -2.889 -2.138
22.366 -3.268 2.848
-3.268 26.165 -0.066
2.848 -0.066 30.274

orbtensor 27 H
4.567 0.311 2.303
0.311 2.600 -2.767
2.303 -2.767 1.172
30.336 -0.221 -1.209
-0.221 21.872 2.971
-1.209 2.971 29.573

orbtensor 28 H
-4.280 -6.107 0.631
-6.107 -15.740 1.510
0.631 1.510 -2.027
31.103 4.858 -1.422
4.858 40.868 -1.614
-1.422 -1.614 22.245

orbtensor 29 H
-18.667 -3.975 2.212
-3.975 -3.031 0.499
2.212 0.499 -3.280
41.473 3.107 -2.712
3.107 30.358 -0.861
-2.712 -0.861 21.927

orbtensor 30 C
-252.190 -11.694 -5.699
-11.694 -88.780 -26.521
-5.699 -26.521 -226.647
258.297 -0.110 -4.724
-0.110 236.050 3.070
-4.724 3.070 261.406

orbtensor 31 H
-1.978 -1.723 -0.589

-1.723	3.149	-0.345
-0.589	-0.345	5.085
34.481	-1.041	-0.904
-1.041	22.765	1.412
-0.904	1.412	25.340

orbtensor 32 H

0.859	-2.033	-3.849
-2.033	4.715	-0.929
-3.849	-0.929	1.518
27.354	2.562	3.684
2.562	24.048	-3.334
3.684	-3.334	28.265

orbtensor 33 H

3.103	-1.110	-0.957
-1.110	3.408	-0.594
-0.957	-0.594	4.554
27.456	5.336	3.034
5.336	29.419	3.259
3.034	3.259	22.705

orbtensor 34 H

-7.009	6.455	0.512
6.455	-13.100	-0.157
0.512	-0.157	-0.338
34.513	-3.379	-1.761
-3.379	34.328	-0.355
-1.761	-0.355	19.600

orbtensor 35 H

-18.925	0.567	2.003
0.567	-2.825	-0.075
2.003	-0.075	-3.258
42.784	-0.638	-2.628
-0.638	30.271	-0.356
-2.628	-0.356	22.308

orbtensor 36 H

-7.772	8.044	0.188
8.044	-12.875	-0.513
0.188	-0.513	-3.004
33.940	-6.969	-1.097
-6.969	38.039	0.074
-1.097	0.074	22.628

orbtensor 37 H

-3.703	-5.788	0.639
-5.788	-16.642	1.558
0.639	1.558	-1.178
30.608	1.977	-1.359
1.977	40.347	-1.281
-1.359	-1.281	21.028

orbtensor 38 Cr

-5899.042	837.148	-189.852
837.148	-3990.001	-268.001
-189.852	-268.001	-7002.128
1801.320	0.524	0.155
0.524	1811.911	-0.548
0.155	-0.548	1802.755

orbtensor 39 Br

-161.295	-18.906	29.967
-18.906	-386.159	65.196
29.967	65.196	-288.264
3095.416	-1.278	-2.164

-1.278 3100.251 5.955
 -2.164 5.955 3101.720

orbtensor 40 Br
 -184.091 -37.644 -52.315
 -37.644 -398.844 -45.724
 -52.315 -45.724 -254.864
 3096.936 -2.398 3.762
 -2.398 3099.069 -5.273
 3.762 -5.273 3101.381

gtensor (ppt)
 -0.173 0.005 0.000
 0.005 -0.156 -0.002
 0.000 -0.002 -0.172
 -0.301 7.721 -2.392
 7.721 -0.456 -1.799
 -2.392 -1.799 -15.438

zfstensor (cm-1)
 -7.725357 -0.168953 0.335224
 -0.168953 -6.056142 0.054549
 0.335224 0.054549 -4.834914

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.5473	-30.37467	6484.67289	-20.78489	6463.88801	6433.51334
2	C	3.5657	13.78967	-1873.39513	1.96517	-1871.42996	-1857.64029
3	C	-1.2960	59.06867	680.91617	-6.01001	674.90616	733.97482
4	C	1.5910	36.02433	-835.90866	5.38708	-830.52158	-794.49725
5	C	-1.5070	48.49900	791.77521	-3.97179	787.80341	836.30241
6	C	0.8077	19.17067	-424.34668	0.36111	-423.98557	-404.81491
7	C	0.8787	49.36833	-461.64996	2.68786	-458.96210	-409.59376
8	C	-0.9867	50.92100	518.39297	-3.11032	515.28265	566.20365
9	C	-0.2510	43.57333	131.87497	3.10966	134.98463	178.55797
10	C	0.2930	42.02100	-153.94170	-4.19332	-158.13502	-116.11402
11	C	-1.5483	61.53667	813.49167	2.61519	816.10686	877.64353
12	C	0.6880	69.07100	-361.47402	3.35514	-358.11888	-289.04788
13	C	0.5563	62.73333	-292.29658	-5.03757	-297.33415	-234.60082
14	C	0.6880	69.12000	-361.47402	3.04412	-358.42989	-289.30989
15	C	0.3747	176.55000	-196.84922	2.68370	-194.16552	-17.61552
16	H	-0.0383	29.88467	5.06535	0.68294	5.74830	35.63296
17	H	0.0170	30.06967	-2.24637	1.38864	-0.85773	29.21194
18	H	-0.2127	28.66400	28.10171	2.83558	30.93728	59.60128
19	C	0.4257	177.05267	-223.64453	-1.71576	-225.36030	-48.30763
20	H	-1.1143	30.23900	147.24765	-0.80875	146.43889	176.67789
21	H	-0.3530	28.92333	46.64531	-0.11950	46.52581	75.44914
22	H	-0.2097	29.63167	27.70529	-2.19506	25.51023	55.14189
23	C	0.4260	177.08333	-223.81967	-1.87359	-225.69325	-48.60992
24	C	0.3750	176.51100	-197.02435	2.60324	-194.42112	-17.91012
25	H	-0.0390	29.85600	5.15345	0.63748	5.79093	35.64693
26	H	-0.2123	28.64233	28.05766	2.76318	30.82084	59.46318
27	H	0.0170	30.04000	-2.24637	1.39327	-0.85310	29.18690
28	H	0.7933	24.05633	-104.83081	-1.08163	-105.91244	-81.85611
29	H	-1.0130	22.92667	133.85750	-0.84459	133.01291	155.93957
30	C	0.5557	62.71200	-291.94631	-5.28467	-297.23098	-234.51898
31	H	-0.2103	29.61400	27.79338	-2.26697	25.52641	55.14041
32	H	-0.3517	28.91967	46.46912	-0.27273	46.19639	75.11606
33	H	-1.1143	30.21500	147.24765	-0.87169	146.37596	176.59096
34	H	-1.1683	22.66467	154.38319	-3.38045	151.00275	173.66741
35	H	-0.5883	23.45167	77.74218	-0.40195	77.34023	100.79189
36	H	0.4353	23.65200	-57.52481	-0.26016	-57.78497	-34.13297
37	H	-0.4413	23.48667	58.31765	0.07914	58.39679	81.88345
38	Cr	35.1617	-3825.06167	82034.83837	33.29200	82068.13037	78243.06871
39	Br	8.2513	2820.55633	-4336.95570	-105.80161	-4442.75731	-1622.20098

40 Br 8.2520 2819.86233 -4337.30610 -106.13093 -4443.43703 -1623.57470

=====
CrL2-STO-BP-No-ZFS
Temperature: 298
Spin: 1.5

atensor 1 N
-1.780 0.249 -0.227
0.249 -2.529 -0.081
-0.227 -0.081 -3.422
0.003 0.014 0.001
0.002 0.012 0.000
0.002 -0.001 0.019

atensor 2 C
2.656 0.978 0.387
0.978 1.915 0.094
0.387 0.094 6.033
-0.059 -0.015 0.009
0.077 0.064 -0.013
0.004 -0.001 0.006

atensor 3 C
0.205 0.180 -0.270
0.180 -0.412 -0.098
-0.270 -0.098 -1.797
0.005 -0.004 0.000
0.006 -0.002 -0.001
-0.001 0.001 0.000

atensor 4 C
0.121 0.097 0.503
0.097 -0.444 0.227
0.503 0.227 4.022
0.002 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.613 -0.080 -0.130
-0.080 -1.074 -0.021
-0.130 -0.021 -1.649
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.056
-0.446 -0.676 0.135
-0.056 0.135 0.811
0.014 -0.011 -0.002
-0.016 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.123 -0.100 0.086
-0.100 -0.149 0.060
0.086 0.060 0.738
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.132 -0.152 -0.069
-0.152 -0.225 -0.007

-0.069 -0.007 -0.725
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.103 -0.248 0.129
-0.248 -0.986 0.073
0.129 0.073 -0.214
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.336 -0.947 -0.170
-0.947 0.942 0.051
-0.170 0.051 -0.368
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.386 -1.501 0.022
-1.501 -1.847 0.286
0.022 0.286 -0.077
0.044 0.002 0.002
0.000 0.010 0.003
0.002 0.002 0.060

atensor 12 C
0.250 -0.484 0.080
-0.484 2.179 -2.299
0.080 -2.299 1.440
0.012 0.013 -0.014
-0.032 0.011 -0.027
-0.006 0.013 0.043

atensor 13 C
1.814 1.602 -0.794
1.602 0.264 -1.054
-0.794 -1.054 1.218
0.023 0.020 -0.008
-0.023 0.028 0.026
0.007 0.003 0.072

atensor 14 C
0.284 0.102 0.179
0.102 2.656 2.220
0.179 2.220 0.929
0.019 0.011 0.018
-0.023 0.013 0.037
0.015 -0.013 0.034

atensor 15 C
-0.021 -0.231 0.311
-0.231 0.385 -0.774
0.311 -0.774 1.053
0.003 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.111 -0.202 0.246
-0.202 1.324 -1.392
0.246 -1.392 1.213
-0.009 0.001 -0.006
-0.004 0.004 -0.010

0.005 0.002 0.001

atensor 17 H
-0.093 -1.206 1.613
-1.206 -0.167 -1.699
1.613 -1.699 0.796
-0.009 -0.008 0.005
-0.011 -0.004 -0.005
0.003 0.005 -0.002

atensor 18 H
-1.804 -0.242 0.521
-0.242 -1.078 -1.733
0.521 -1.733 2.903
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.008 -0.004

atensor 19 C
0.507 0.431 -0.603
0.431 0.104 -0.391
-0.603 -0.391 0.455
0.002 0.001 -0.003
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.699 0.935 -0.820
0.935 -0.530 -0.868
-0.820 -0.868 -0.785
0.006 0.007 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.334 0.839 -2.146
0.838 -1.411 -1.090
-2.146 -1.090 1.159
0.002 0.000 -0.023
0.007 0.001 -0.015
-0.002 0.007 0.000

atensor 22 H
1.502 1.174 -1.475
1.174 -1.091 -0.598
-1.475 -0.598 -0.787
0.017 0.001 -0.012
0.010 0.001 -0.006
-0.005 0.001 0.000

atensor 23 C
0.784 0.575 0.454
0.575 0.176 0.276
0.454 0.276 0.108
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.104 -0.038 -0.018
-0.038 0.557 0.868
-0.018 0.868 0.962
0.004 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H

-0.152 0.143 0.074
0.143 1.614 1.362
0.074 1.362 0.962
-0.008 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.767 0.259 0.642
0.259 -0.673 2.114
0.642 2.114 2.460
-0.017 -0.009 0.010
-0.003 -0.001 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.801 -0.872 -1.135
-0.872 0.229 2.066
-1.135 2.066 1.108
-0.010 -0.010 -0.002
-0.010 -0.004 0.008
0.000 -0.003 -0.001

atensor 28 H
1.416 0.649 -0.224
0.649 0.551 -0.116
-0.224 -0.116 -0.034
0.008 0.002 -0.001
0.010 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
-0.068 0.351 -0.224
0.351 -2.465 -0.004
-0.224 -0.003 -1.650
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.113 1.886 0.348
1.886 0.446 0.669
0.348 0.669 0.734
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.040 1.396 0.588
1.396 -1.000 0.256
0.588 0.256 -1.417
0.020 0.002 0.007
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.774 1.338 2.100
1.338 -1.186 1.000
2.100 1.000 -0.172
0.008 0.001 0.021
0.010 0.002 0.012
-0.001 -0.008 -0.007

atensor 33 H
-0.335 1.191 0.568
1.191 -0.381 0.532
0.568 0.532 -1.297

0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.548 2.877 -0.468
2.877 0.625 -0.612
-0.468 -0.612 -3.932
0.036 0.067 -0.006
0.014 -0.008 -0.001
-0.003 -0.007 0.016

atensor 35 H
0.210 -0.258 -0.107
-0.258 -0.732 0.033
-0.107 0.033 -0.720
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.360 -0.363 -0.056
-0.363 0.126 0.028
-0.056 0.028 -0.218
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.509 -0.625 -0.002
-0.625 0.506 0.012
-0.002 0.012 -0.785
-0.006 -0.005 0.001
-0.007 0.000 0.001
0.001 0.001 0.000

atensor 38 Cr
17.601 2.573 -0.264
2.573 26.950 -0.873
-0.264 -0.873 16.672
0.135 -0.805 0.320
-0.822 0.696 0.190
0.320 0.188 2.254

atensor 39 Br
31.683 1.582 10.767
1.582 11.957 -26.862
10.767 -26.862 -29.055
-1.251 -0.263 -0.514
-0.241 -0.149 2.582
-0.835 2.030 3.032

atensor 40 Br
22.422 5.827 -25.230
5.827 17.041 21.425
-25.230 21.425 -24.860
-0.633 -0.610 1.574
-0.695 -0.585 -2.105
1.897 -1.562 2.849

orbtensor 1 N
-479.333 53.189 47.189
53.189 -548.972 17.432
47.189 17.432 -95.265
338.750 -3.782 -2.113
-3.782 349.694 -1.043
-2.113 -1.043 320.986

orbtensor 2 C
-272.809 26.350 24.450
26.350 -297.960 8.582
24.450 8.582 -74.283
253.140 5.817 -5.648
5.817 251.785 -2.870
-5.648 -2.870 212.225

orbtensor 3 C
-219.895 -44.596 23.617
-44.596 -287.516 18.008
23.617 18.008 -57.452
252.431 3.307 -3.936
3.307 262.817 -2.517
-3.936 -2.517 223.635

orbtensor 4 C
-300.053 -23.695 32.688
-23.695 -232.997 12.439
32.688 12.439 -58.897
257.114 3.196 -5.255
3.196 253.215 -2.296
-5.255 -2.296 218.111

orbtensor 5 C
-287.857 2.875 29.647
2.875 -275.754 11.256
29.647 11.256 -59.098
269.113 0.365 -4.437
0.365 266.708 -1.738
-4.437 -1.738 235.207

orbtensor 6 C
-275.044 20.815 21.501
20.815 -296.206 7.749
21.501 7.749 -101.448
263.417 -5.183 -5.606
-5.183 261.096 -1.634
-5.606 -1.634 218.229

orbtensor 7 C
-296.781 10.290 30.102
10.290 -210.225 6.740
30.102 6.740 -61.200
258.100 -4.153 -4.984
-4.153 251.935 -1.285
-4.984 -1.285 218.097

orbtensor 8 C
-251.026 54.691 23.089
54.691 -268.125 4.587
23.089 4.587 -51.080
253.974 -5.686 -4.066
-5.686 255.806 -1.164
-4.066 -1.164 220.408

orbtensor 9 C
-234.354 -33.807 24.709
-33.807 -292.005 16.784
24.709 16.784 -59.002
253.150 -3.842 -4.172
-3.842 257.439 -1.533
-4.172 -1.533 219.543

orbtensor 10 C
-301.449 -15.850 28.358

-15.850	-249.921	10.636
28.358	10.636	-90.345
270.045	-1.183	-4.404
-1.183	264.970	-1.418
-4.404	-1.418	235.754

orbtensor 11 C

-219.922	31.186	-0.217
31.186	-131.627	-8.047
-0.217	-8.047	-208.332
248.019	-8.521	-1.124
-8.521	240.516	0.838
-1.124	0.838	235.823

orbtensor 12 C

-200.628	18.143	0.026
18.143	-105.442	24.269
0.026	24.269	-235.524
242.234	-2.874	-4.259
-2.874	236.428	-6.608
-4.259	-6.608	244.318

orbtensor 13 C

-227.692	-8.985	14.047
-8.985	-94.145	13.453
14.047	13.453	-220.105
245.616	4.710	-1.981
4.710	233.904	-4.384
-1.981	-4.384	244.418

orbtensor 14 C

-203.121	9.290	-9.134
9.290	-112.316	-40.723
-9.134	-40.723	-226.148
244.462	-0.585	4.218
-0.585	237.938	7.607
4.218	7.607	240.584

orbtensor 15 C

-57.332	0.543	6.355
0.543	-48.186	2.910
6.355	2.910	-50.683
219.030	-0.666	2.806
-0.666	218.693	-4.285
2.806	-4.285	228.230

orbtensor 16 H

3.192	-0.656	0.002
-0.656	1.940	1.387
0.002	1.387	1.457
23.260	0.390	-0.238
0.390	29.612	-6.893
-0.238	-6.893	29.170

orbtensor 17 H

3.294	0.444	-2.082
0.444	3.502	2.321
-2.082	2.321	2.843
30.083	-0.359	0.652
-0.359	21.044	-2.433
0.652	-2.433	28.631

orbtensor 18 H

5.077	0.385	-0.146
0.385	3.246	2.179
-0.146	2.179	-1.283
21.126	-3.178	-0.400

-3.178 27.066 0.765
-0.400 0.765 30.090

orbtensor 19 C
-54.843 -0.471 -5.693
-0.471 -46.380 2.391
-5.693 2.391 -55.903
225.951 1.630 -6.830
1.630 219.190 -1.578
-6.830 -1.578 223.277

orbtensor 20 H
2.293 -0.623 1.098
-0.623 1.987 0.842
1.098 0.842 2.438
26.454 3.911 -3.980
3.911 29.332 -5.110
-3.980 -5.110 26.292

orbtensor 21 H
2.660 -1.614 2.721
-1.614 3.503 1.035
2.721 1.035 0.244
25.264 3.565 -3.063
3.565 25.439 2.708
-3.063 2.708 28.488

orbtensor 22 H
-0.917 -1.127 1.403
-1.127 2.954 1.218
1.403 1.218 3.693
33.480 -1.393 -0.791
-1.393 22.747 -1.384
-0.791 -1.384 25.652

orbtensor 23 C
-52.116 -0.634 4.839
-0.634 -46.984 -3.340
4.839 -3.340 -58.035
229.046 2.642 5.057
2.642 219.501 1.253
5.057 1.253 219.873

orbtensor 24 C
-59.997 -0.761 -3.842
-0.761 -48.812 -2.923
-3.842 -2.923 -47.400
218.235 0.394 -0.317
0.394 219.700 5.279
-0.317 5.279 228.018

orbtensor 25 H
3.106 -1.005 -0.306
-1.005 1.667 -1.194
-0.306 -1.194 1.814
23.694 2.181 1.340
2.181 31.010 6.354
1.340 6.354 27.338

orbtensor 26 H
4.752 -0.296 -1.364
-0.296 2.739 -2.609
-1.364 -2.609 -0.453
21.968 -3.057 2.856
-3.057 27.025 0.330
2.856 0.330 29.286

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orbtensor 27 H
4.280    0.039    1.746
0.039    2.999   -2.454
1.746   -2.454    2.356
29.667    0.274   -0.988
0.274    21.638    3.202
-0.988    3.202   28.454

orbtensor 28 H
-5.449   -5.922    0.661
-5.922  -16.876    1.501
0.661    1.501   -2.879
32.070    4.818   -1.360
4.818   41.590   -1.572
-1.360   -1.572   23.668

orbtensor 29 H
-18.290   -3.039    2.292
-3.039   -3.599    0.493
2.292    0.493   -1.924
41.651    2.416   -2.732
2.416   30.576   -0.798
-2.732   -0.798   21.663

orbtensor 30 C
-233.681  -14.896   -8.798
-14.896  -98.004  -22.932
-8.798   -22.932 -210.238
246.347    5.936    0.790
5.936   234.785    3.988
0.790    3.988   242.791

orbtensor 31 H
-1.270   -1.455    0.056
-1.455    2.743   -0.759
0.056   -0.759    4.256
33.395   -0.985   -1.136
-0.985   23.102    1.950
-1.136    1.950   25.383

orbtensor 32 H
1.235   -2.148   -2.748
-2.148    3.303   -0.801
-2.748   -0.801    1.866
26.882    3.137    3.198
3.137   24.809   -3.262
3.198   -3.262   27.502

orbtensor 33 H
1.789   -0.908   -0.826
-0.908    1.837   -0.552
-0.826   -0.552    3.090
28.245    5.380    2.845
5.380   30.237    3.396
2.845    3.396   23.597

orbtensor 34 H
-8.513    4.270    0.722
4.270   -13.818    0.122
0.722    0.122   -1.208
35.528   -1.286   -1.907
-1.286   34.985   -0.619
-1.907   -0.619   20.363

orbtensor 35 H
-18.305    0.194    2.079
0.194   -3.345    0.048

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2.079 0.048 -2.224
42.253 -0.368 -2.633
-0.368 30.338 -0.418
-2.633 -0.418 21.860

orbtensor 36 H
-8.516 7.871 0.264
7.871 -13.242 -0.478
0.264 -0.478 -3.218
34.452 -6.970 -1.067
-6.970 38.072 0.111
-1.067 0.111 23.368

orbtensor 37 H
-4.881 -4.747 0.679
-4.747 -16.705 1.405
0.679 1.405 -1.688
31.365 1.205 -1.286
1.205 40.413 -1.132
-1.286 -1.132 22.025

orbtensor 38 Cr
-5040.523 401.164 -78.879
401.164 -3571.210 -152.519
-78.879 -152.519 -5474.863
1810.105 -0.348 0.235
-0.348 1811.894 0.041
0.235 0.041 1811.770

orbtensor 39 Br
-872.955 -63.954 -2.676
-63.954 -1078.710 449.779
-2.676 449.779 -931.661
3090.062 -1.761 -3.348
-1.761 3096.688 8.392
-3.348 8.392 3099.539

orbtensor 40 Br
-870.735 -171.804 11.366
-171.804 -1167.968 -394.655
11.366 -394.655 -844.601
3092.386 -3.294 5.700
-3.294 3095.028 -7.374
5.700 -7.374 3098.875

gtensor (ppt)
-0.154 0.005 0.000
0.005 -0.156 -0.001
0.000 -0.001 -0.155
14.173 8.034 -1.802
8.034 13.646 -1.568
-1.802 -1.568 3.701

averaging
2H Average:34
4H Average:29
9,10H Average:16,17,18,20,21,22
5H Average:35
8,11H Average:25,26,27,31,32,33
6H Average:36
3H Average:28
7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
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1	N	-2.5657	-38.04667	4727.41748	-4.25521	4723.16227	4685.11560
2	C	3.5383	24.03267	-1873.80780	0.95013	-1872.85767	-1848.82500
3	C	-0.6670	58.00667	353.22557	-1.39394	351.83163	409.83830
4	C	1.2263	45.49767	-649.43372	2.57704	-646.85668	-601.35901
5	C	-1.1093	49.43967	587.47361	-0.42579	587.04782	636.48749
6	C	0.5177	23.34800	-274.14258	0.87773	-273.26486	-249.91686
7	C	0.2357	53.30867	-124.80284	0.62885	-124.17399	-70.86532
8	C	-0.3597	53.31900	190.46996	-0.14084	190.32912	243.64812
9	C	-0.7720	48.25700	408.83079	0.92704	409.75784	458.01484
10	C	0.6347	43.01800	-336.10269	0.40273	-335.69996	-292.68196
11	C	-0.4747	54.82567	251.37092	2.55939	253.93031	308.75598
12	C	1.3117	60.46200	-694.62399	0.28150	-694.34249	-633.88049
13	C	1.1397	60.66533	-603.53734	-2.69541	-606.23275	-545.56742
14	C	1.3117	60.46633	-694.62399	0.28343	-694.34056	-633.87423
15	C	0.4753	169.91733	-251.72397	0.74322	-250.98075	-81.06341
16	H	0.8073	29.54367	-107.52855	0.09508	-107.43347	-77.88980
17	H	0.1737	29.79900	-23.13063	0.58132	-22.54931	7.24969
18	H	-0.0003	28.44067	0.04440	0.66686	0.71125	29.15192
19	C	0.3597	170.43067	-190.46996	-0.82416	-191.29412	-20.86346
20	H	-0.6677	29.59867	88.92638	-0.48493	88.44145	118.04012
21	H	-0.1943	28.53267	25.88321	-0.24749	25.63573	54.16839
22	H	-0.1193	29.20300	15.89398	-0.74339	15.15059	44.35359
23	C	0.3603	170.42833	-190.82301	-0.82535	-191.64836	-21.22002
24	C	0.4747	169.91467	-251.37092	0.74384	-250.62708	-80.71241
25	H	0.8067	29.54300	-107.43976	0.09545	-107.34430	-77.80130
26	H	-0.0013	28.43900	0.17759	0.66750	0.84508	29.28408
27	H	0.1737	29.79800	-23.13063	0.58189	-22.54873	7.24927
28	H	0.6493	24.04133	-86.48456	-0.41674	-86.90131	-62.85997
29	H	-1.3933	23.35900	185.57776	-0.21402	185.36374	208.72274
30	C	1.1387	60.66667	-603.00777	-2.69542	-605.70319	-545.03652
31	H	-0.1193	29.20300	15.89398	-0.74337	15.15061	44.35361
32	H	-0.1937	28.53233	25.79442	-0.24755	25.54687	54.07921
33	H	-0.6673	29.59833	88.88198	-0.48491	88.39707	117.99540
34	H	-1.6037	22.44567	213.59201	-1.62320	211.96881	234.41448
35	H	-0.4133	23.52567	55.05178	0.01145	55.06323	78.58890
36	H	0.0890	23.63867	-11.85389	0.05643	-11.79746	11.84121
37	H	-0.2647	23.50967	35.25089	0.11340	35.36429	58.87396
38	Cr	21.4360	-2884.27567	50409.25443	20.73373	50429.98816	47545.71249
39	Br	5.4057	2134.32100	-2863.83352	-34.02898	-2897.86249	-763.54149
40	Br	5.4113	2134.32833	-2866.83562	-34.02112	-2900.85674	-766.52841

=====
CrL2-STO-BP-Neese
Temperature: 298
Spin: 1.5

atensor 1 N
-1.780 0.249 -0.227
0.249 -2.529 -0.081
-0.227 -0.081 -3.422
0.003 0.014 0.001
0.002 0.012 0.000
0.002 -0.001 0.019

atensor 2 C
2.656 0.978 0.387
0.978 1.915 0.094
0.387 0.094 6.033
-0.059 -0.015 0.009
0.077 0.064 -0.013
0.004 -0.001 0.006

atensor 3 C
0.205 0.180 -0.270
0.180 -0.412 -0.098

-0.270 -0.098 -1.797
0.005 -0.004 0.000
0.006 -0.002 -0.001
-0.001 0.001 0.000

atensor 4 C
0.121 0.097 0.503
0.097 -0.444 0.227
0.503 0.227 4.022
0.002 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.613 -0.080 -0.130
-0.080 -1.074 -0.021
-0.130 -0.021 -1.649
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.056
-0.446 -0.676 0.135
-0.056 0.135 0.811
0.014 -0.011 -0.002
-0.016 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.123 -0.100 0.086
-0.100 -0.149 0.060
0.086 0.060 0.738
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.132 -0.152 -0.069
-0.152 -0.225 -0.007
-0.069 -0.007 -0.725
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.103 -0.248 0.129
-0.248 -0.986 0.073
0.129 0.073 -0.214
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.336 -0.947 -0.170
-0.947 0.942 0.051
-0.170 0.051 -0.368
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.386 -1.501 0.022
-1.501 -1.847 0.286
0.022 0.286 -0.077
0.044 0.002 0.002
0.000 0.010 0.003

0.002 0.002 0.060

atensor 12 C
0.250 -0.484 0.080
-0.484 2.179 -2.299
0.080 -2.299 1.440
0.012 0.013 -0.014
-0.032 0.011 -0.027
-0.006 0.013 0.043

atensor 13 C
1.814 1.602 -0.794
1.602 0.264 -1.054
-0.794 -1.054 1.218
0.023 0.020 -0.008
-0.023 0.028 0.026
0.007 0.003 0.072

atensor 14 C
0.284 0.102 0.179
0.102 2.656 2.220
0.179 2.220 0.929
0.019 0.011 0.018
-0.023 0.013 0.037
0.015 -0.013 0.034

atensor 15 C
-0.021 -0.231 0.311
-0.231 0.385 -0.774
0.311 -0.774 1.053
0.003 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.111 -0.202 0.246
-0.202 1.324 -1.392
0.246 -1.392 1.213
-0.009 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.093 -1.206 1.613
-1.206 -0.167 -1.699
1.613 -1.699 0.796
-0.009 -0.008 0.005
-0.011 -0.004 -0.005
0.003 0.005 -0.002

atensor 18 H
-1.804 -0.242 0.521
-0.242 -1.078 -1.733
0.521 -1.733 2.903
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.008 -0.004

atensor 19 C
0.507 0.431 -0.603
0.431 0.104 -0.391
-0.603 -0.391 0.455
0.002 0.001 -0.003
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H

-0.699 0.935 -0.820
0.935 -0.530 -0.868
-0.820 -0.868 -0.785
0.006 0.007 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.334 0.839 -2.146
0.838 -1.411 -1.090
-2.146 -1.090 1.159
0.002 0.000 -0.023
0.007 0.001 -0.015
-0.002 0.007 0.000

atensor 22 H
1.502 1.174 -1.475
1.174 -1.091 -0.598
-1.475 -0.598 -0.787
0.017 0.001 -0.012
0.010 0.001 -0.006
-0.005 0.001 0.000

atensor 23 C
0.784 0.575 0.454
0.575 0.176 0.276
0.454 0.276 0.108
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.104 -0.038 -0.018
-0.038 0.557 0.868
-0.018 0.868 0.962
0.004 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.152 0.143 0.074
0.143 1.614 1.362
0.074 1.362 0.962
-0.008 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.767 0.259 0.642
0.259 -0.673 2.114
0.642 2.114 2.460
-0.017 -0.009 0.010
-0.003 -0.001 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.801 -0.872 -1.135
-0.872 0.229 2.066
-1.135 2.066 1.108
-0.010 -0.010 -0.002
-0.010 -0.004 0.008
0.000 -0.003 -0.001

atensor 28 H
1.416 0.649 -0.224
0.649 0.551 -0.116
-0.224 -0.116 -0.034

0.008 0.002 -0.001
0.010 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
-0.068 0.351 -0.224
0.351 -2.465 -0.004
-0.224 -0.003 -1.650
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.113 1.886 0.348
1.886 0.446 0.669
0.348 0.669 0.734
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.040 1.396 0.588
1.396 -1.000 0.256
0.588 0.256 -1.417
0.020 0.002 0.007
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.774 1.338 2.100
1.338 -1.186 1.000
2.100 1.000 -0.172
0.008 0.001 0.021
0.010 0.002 0.012
-0.001 -0.008 -0.007

atensor 33 H
-0.335 1.191 0.568
1.191 -0.381 0.532
0.568 0.532 -1.297
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.548 2.877 -0.468
2.877 0.625 -0.612
-0.468 -0.612 -3.932
0.036 0.067 -0.006
0.014 -0.008 -0.001
-0.003 -0.007 0.016

atensor 35 H
0.210 -0.258 -0.107
-0.258 -0.732 0.033
-0.107 0.033 -0.720
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.360 -0.363 -0.056
-0.363 0.126 0.028
-0.056 0.028 -0.218
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.509 -0.625 -0.002
-0.625 0.506 0.012
-0.002 0.012 -0.785
-0.006 -0.005 0.001
-0.007 0.000 0.001
0.001 0.001 0.000

atensor 38 Cr
17.601 2.573 -0.264
2.573 26.950 -0.873
-0.264 -0.873 16.672
0.135 -0.805 0.320
-0.822 0.696 0.190
0.320 0.188 2.254

atensor 39 Br
31.683 1.582 10.767
1.582 11.957 -26.862
10.767 -26.862 -29.055
-1.251 -0.263 -0.514
-0.241 -0.149 2.582
-0.835 2.030 3.032

atensor 40 Br
22.422 5.827 -25.230
5.827 17.041 21.425
-25.230 21.425 -24.860
-0.633 -0.610 1.574
-0.695 -0.585 -2.105
1.897 -1.562 2.849

orbtensor 1 N
-479.333 53.189 47.189
53.189 -548.972 17.432
47.189 17.432 -95.265
338.750 -3.782 -2.113
-3.782 349.694 -1.043
-2.113 -1.043 320.986

orbtensor 2 C
-272.809 26.350 24.450
26.350 -297.960 8.582
24.450 8.582 -74.283
253.140 5.817 -5.648
5.817 251.785 -2.870
-5.648 -2.870 212.225

orbtensor 3 C
-219.895 -44.596 23.617
-44.596 -287.516 18.008
23.617 18.008 -57.452
252.431 3.307 -3.936
3.307 262.817 -2.517
-3.936 -2.517 223.635

orbtensor 4 C
-300.053 -23.695 32.688
-23.695 -232.997 12.439
32.688 12.439 -58.897
257.114 3.196 -5.255
3.196 253.215 -2.296
-5.255 -2.296 218.111

orbtensor 5 C
-287.857 2.875 29.647

2.875	-275.754	11.256
29.647	11.256	-59.098
269.113	0.365	-4.437
0.365	266.708	-1.738
-4.437	-1.738	235.207

orbtensor 6 C

-275.044	20.815	21.501
20.815	-296.206	7.749
21.501	7.749	-101.448
263.417	-5.183	-5.606
-5.183	261.096	-1.634
-5.606	-1.634	218.229

orbtensor 7 C

-296.781	10.290	30.102
10.290	-210.225	6.740
30.102	6.740	-61.200
258.100	-4.153	-4.984
-4.153	251.935	-1.285
-4.984	-1.285	218.097

orbtensor 8 C

-251.026	54.691	23.089
54.691	-268.125	4.587
23.089	4.587	-51.080
253.974	-5.686	-4.066
-5.686	255.806	-1.164
-4.066	-1.164	220.408

orbtensor 9 C

-234.354	-33.807	24.709
-33.807	-292.005	16.784
24.709	16.784	-59.002
253.150	-3.842	-4.172
-3.842	257.439	-1.533
-4.172	-1.533	219.543

orbtensor 10 C

-301.449	-15.850	28.358
-15.850	-249.921	10.636
28.358	10.636	-90.345
270.045	-1.183	-4.404
-1.183	264.970	-1.418
-4.404	-1.418	235.754

orbtensor 11 C

-219.922	31.186	-0.217
31.186	-131.627	-8.047
-0.217	-8.047	-208.332
248.019	-8.521	-1.124
-8.521	240.516	0.838
-1.124	0.838	235.823

orbtensor 12 C

-200.628	18.143	0.026
18.143	-105.442	24.269
0.026	24.269	-235.524
242.234	-2.874	-4.259
-2.874	236.428	-6.608
-4.259	-6.608	244.318

orbtensor 13 C

-227.692	-8.985	14.047
-8.985	-94.145	13.453
14.047	13.453	-220.105
245.616	4.710	-1.981

4.710	233.904	-4.384
-1.981	-4.384	244.418

orbtensor 14 C

-203.121	9.290	-9.134
9.290	-112.316	-40.723
-9.134	-40.723	-226.148
244.462	-0.585	4.218
-0.585	237.938	7.607
4.218	7.607	240.584

orbtensor 15 C

-57.332	0.543	6.355
0.543	-48.186	2.910
6.355	2.910	-50.683
219.030	-0.666	2.806
-0.666	218.693	-4.285
2.806	-4.285	228.230

orbtensor 16 H

3.192	-0.656	0.002
-0.656	1.940	1.387
0.002	1.387	1.457
23.260	0.390	-0.238
0.390	29.612	-6.893
-0.238	-6.893	29.170

orbtensor 17 H

3.294	0.444	-2.082
0.444	3.502	2.321
-2.082	2.321	2.843
30.083	-0.359	0.652
-0.359	21.044	-2.433
0.652	-2.433	28.631

orbtensor 18 H

5.077	0.385	-0.146
0.385	3.246	2.179
-0.146	2.179	-1.283
21.126	-3.178	-0.400
-3.178	27.066	0.765
-0.400	0.765	30.090

orbtensor 19 C

-54.843	-0.471	-5.693
-0.471	-46.380	2.391
-5.693	2.391	-55.903
225.951	1.630	-6.830
1.630	219.190	-1.578
-6.830	-1.578	223.277

orbtensor 20 H

2.293	-0.623	1.098
-0.623	1.987	0.842
1.098	0.842	2.438
26.454	3.911	-3.980
3.911	29.332	-5.110
-3.980	-5.110	26.292

orbtensor 21 H

2.660	-1.614	2.721
-1.614	3.503	1.035
2.721	1.035	0.244
25.264	3.565	-3.063
3.565	25.439	2.708
-3.063	2.708	28.488

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orbtensor 22 H
-0.917  -1.127   1.403
-1.127   2.954   1.218
 1.403   1.218   3.693
33.480  -1.393  -0.791
-1.393  22.747  -1.384
-0.791  -1.384  25.652

orbtensor 23 C
-52.116  -0.634   4.839
-0.634  -46.984  -3.340
 4.839  -3.340 -58.035
229.046   2.642   5.057
 2.642 219.501   1.253
 5.057   1.253 219.873

orbtensor 24 C
-59.997  -0.761  -3.842
-0.761 -48.812  -2.923
-3.842 -2.923 -47.400
218.235   0.394  -0.317
 0.394 219.700   5.279
-0.317   5.279 228.018

orbtensor 25 H
 3.106  -1.005  -0.306
-1.005   1.667  -1.194
-0.306  -1.194   1.814
23.694   2.181   1.340
 2.181 31.010   6.354
 1.340   6.354 27.338

orbtensor 26 H
 4.752  -0.296  -1.364
-0.296   2.739  -2.609
-1.364  -2.609  -0.453
21.968  -3.057   2.856
-3.057  27.025   0.330
 2.856   0.330 29.286

orbtensor 27 H
 4.280   0.039   1.746
 0.039   2.999  -2.454
 1.746  -2.454   2.356
29.667   0.274  -0.988
 0.274 21.638   3.202
-0.988   3.202 28.454

orbtensor 28 H
-5.449  -5.922   0.661
-5.922 -16.876   1.501
 0.661   1.501  -2.879
32.070   4.818  -1.360
 4.818 41.590  -1.572
-1.360  -1.572 23.668

orbtensor 29 H
-18.290  -3.039   2.292
-3.039  -3.599   0.493
 2.292   0.493  -1.924
41.651   2.416  -2.732
 2.416 30.576  -0.798
-2.732  -0.798 21.663

orbtensor 30 C
-233.681  -14.896  -8.798
-14.896  -98.004 -22.932

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-8.798	-22.932	-210.238
246.347	5.936	0.790
5.936	234.785	3.988
0.790	3.988	242.791

orbtensor 31 H

-1.270	-1.455	0.056
-1.455	2.743	-0.759
0.056	-0.759	4.256
33.395	-0.985	-1.136
-0.985	23.102	1.950
-1.136	1.950	25.383

orbtensor 32 H

1.235	-2.148	-2.748
-2.148	3.303	-0.801
-2.748	-0.801	1.866
26.882	3.137	3.198
3.137	24.809	-3.262
3.198	-3.262	27.502

orbtensor 33 H

1.789	-0.908	-0.826
-0.908	1.837	-0.552
-0.826	-0.552	3.090
28.245	5.380	2.845
5.380	30.237	3.396
2.845	3.396	23.597

orbtensor 34 H

-8.513	4.270	0.722
4.270	-13.818	0.122
0.722	0.122	-1.208
35.528	-1.286	-1.907
-1.286	34.985	-0.619
-1.907	-0.619	20.363

orbtensor 35 H

-18.305	0.194	2.079
0.194	-3.345	0.048
2.079	0.048	-2.224
42.253	-0.368	-2.633
-0.368	30.338	-0.418
-2.633	-0.418	21.860

orbtensor 36 H

-8.516	7.871	0.264
7.871	-13.242	-0.478
0.264	-0.478	-3.218
34.452	-6.970	-1.067
-6.970	38.072	0.111
-1.067	0.111	23.368

orbtensor 37 H

-4.881	-4.747	0.679
-4.747	-16.705	1.405
0.679	1.405	-1.688
31.365	1.205	-1.286
1.205	40.413	-1.132
-1.286	-1.132	22.025

orbtensor 38 Cr

-5040.523	401.164	-78.879
401.164	-3571.210	-152.519
-78.879	-152.519	-5474.863
1810.105	-0.348	0.235
-0.348	1811.894	0.041

0.235 0.041 1811.770

orbtensor 39 Br

-872.955 -63.954 -2.676
-63.954 -1078.710 449.779
-2.676 449.779 -931.661
3090.062 -1.761 -3.348
-1.761 3096.688 8.392
-3.348 8.392 3099.539

orbtensor 40 Br

-870.735 -171.804 11.366
-171.804 -1167.968 -394.655
11.366 -394.655 -844.601
3092.386 -3.294 5.700
-3.294 3095.028 -7.374
5.700 -7.374 3098.875

gtensor (ppt)

-0.154 0.005 0.000
0.005 -0.156 -0.001
0.000 -0.001 -0.155
14.173 8.034 -1.802
8.034 13.646 -1.568
-1.802 -1.568 3.701

zfstensor (cm-1)

-2.150973 0.776771 0.689966
0.776771 -0.674454 -0.289592
0.689966 -0.289592 2.825427

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.5657	-38.04667	4727.50058	-18.32282	4709.17776	4671.13110
2	C	3.5383	24.03267	-1873.84074	13.38886	-1860.45188	-1836.41921
3	C	-0.6670	58.00667	353.23178	-6.78826	346.44352	404.45019
4	C	1.2263	45.49767	-649.44513	14.93523	-634.50990	-589.01223
5	C	-1.1093	49.43967	587.48394	-3.40550	584.07844	633.51810
6	C	0.5177	23.34800	-274.14740	-0.38631	-274.53372	-251.18572
7	C	0.2357	53.30867	-124.80503	2.51590	-122.28913	-68.98047
8	C	-0.3597	53.31900	190.47331	-2.11871	188.35460	241.67360
9	C	-0.7720	48.25700	408.83798	3.15719	411.99517	460.25217
10	C	0.6347	43.01800	-336.10860	-6.01370	-342.12230	-299.10430
11	C	-0.4747	54.82567	251.37534	0.31629	251.69163	306.51730
12	C	1.3117	60.46200	-694.63620	3.16414	-691.47206	-631.01006
13	C	1.1397	60.66533	-603.54795	-1.19034	-604.73828	-544.07295
14	C	1.3117	60.46633	-694.63620	-0.32621	-694.96241	-634.49608
15	C	0.4753	169.91733	-251.72839	4.08392	-247.64448	-77.72714
16	H	0.8073	29.54367	-107.53044	1.02654	-106.50390	-76.96023
17	H	0.1737	29.79900	-23.13103	1.58492	-21.54612	8.25288
18	H	-0.0003	28.44067	0.04440	4.30453	4.34893	32.78960
19	C	0.3597	170.43067	-190.47331	-0.62514	-191.09845	-20.66778
20	H	-0.6677	29.59867	88.92794	-0.36861	88.55933	118.15800
21	H	-0.1943	28.53267	25.88367	0.75184	26.63551	55.16818
22	H	-0.1193	29.20300	15.89426	-1.93325	13.96101	43.16401
23	C	0.3603	170.42833	-190.82636	-0.96185	-191.78822	-21.35988
24	C	0.4747	169.91467	-251.37534	2.76387	-248.61147	-78.69680
25	H	0.8067	29.54300	-107.44164	0.48356	-106.95808	-77.41508
26	H	-0.0013	28.43900	0.17759	3.56207	3.73966	32.17866
27	H	0.1737	29.79800	-23.13103	0.73375	-22.39728	7.40072
28	H	0.6493	24.04133	-86.48608	-1.12490	-87.61098	-63.56965
29	H	-1.3933	23.35900	185.58102	-0.89012	184.69090	208.04990
30	C	1.1387	60.66667	-603.01837	-2.30927	-605.32764	-544.66097
31	H	-0.1193	29.20300	15.89426	-2.01151	13.88275	43.08575
32	H	-0.1937	28.53233	25.79487	0.52579	26.32066	54.85299

33	H	-0.6673	29.59833	88.88354	-0.58223	88.30131	117.89964
34	H	-1.6037	22.44567	213.59576	-2.64879	210.94697	233.39264
35	H	-0.4133	23.52567	55.05274	-0.64701	54.40573	77.93140
36	H	0.0890	23.63867	-11.85410	-0.49107	-12.34517	11.29350
37	H	-0.2647	23.50967	35.25151	-0.51096	34.74056	58.25022
38	Cr	21.4360	-2884.27567	50410.14054	21.12768	50431.26823	47546.99256
39	Br	5.4057	2134.32100	-2863.88386	-153.21491	-3017.09877	-882.77777
40	Br	5.4113	2134.32833	-2866.88602	-193.15078	-3060.03680	-925.70847

=====
 CrI2-STO-BP-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 N
 -1.780 0.249 -0.227
 0.249 -2.529 -0.081
 -0.227 -0.081 -3.422
 0.003 0.014 0.001
 0.002 0.012 0.000
 0.002 -0.001 0.019

atensor 2 C
 2.656 0.978 0.387
 0.978 1.915 0.094
 0.387 0.094 6.033
 -0.059 -0.015 0.009
 0.077 0.064 -0.013
 0.004 -0.001 0.006

atensor 3 C
 0.205 0.180 -0.270
 0.180 -0.412 -0.098
 -0.270 -0.098 -1.797
 0.005 -0.004 0.000
 0.006 -0.002 -0.001
 -0.001 0.001 0.000

atensor 4 C
 0.121 0.097 0.503
 0.097 -0.444 0.227
 0.503 0.227 4.022
 0.002 0.010 -0.001
 -0.015 -0.021 0.003
 0.000 0.000 -0.001

atensor 5 C
 -0.613 -0.080 -0.130
 -0.080 -1.074 -0.021
 -0.130 -0.021 -1.649
 0.003 -0.003 0.000
 0.000 0.005 0.000
 0.000 0.000 0.000

atensor 6 C
 1.436 -0.446 -0.056
 -0.446 -0.676 0.135
 -0.056 0.135 0.811
 0.014 -0.011 -0.002
 -0.016 -0.029 0.003
 -0.001 0.003 -0.003

atensor 7 C
 0.123 -0.100 0.086
 -0.100 -0.149 0.060
 0.086 0.060 0.738

0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.132 -0.152 -0.069
-0.152 -0.225 -0.007
-0.069 -0.007 -0.725
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.103 -0.248 0.129
-0.248 -0.986 0.073
0.129 0.073 -0.214
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.336 -0.947 -0.170
-0.947 0.942 0.051
-0.170 0.051 -0.368
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.386 -1.501 0.022
-1.501 -1.847 0.286
0.022 0.286 -0.077
0.044 0.002 0.002
0.000 0.010 0.003
0.002 0.002 0.060

atensor 12 C
0.250 -0.484 0.080
-0.484 2.179 -2.299
0.080 -2.299 1.440
0.012 0.013 -0.014
-0.032 0.011 -0.027
-0.006 0.013 0.043

atensor 13 C
1.814 1.602 -0.794
1.602 0.264 -1.054
-0.794 -1.054 1.218
0.023 0.020 -0.008
-0.023 0.028 0.026
0.007 0.003 0.072

atensor 14 C
0.284 0.102 0.179
0.102 2.656 2.220
0.179 2.220 0.929
0.019 0.011 0.018
-0.023 0.013 0.037
0.015 -0.013 0.034

atensor 15 C
-0.021 -0.231 0.311
-0.231 0.385 -0.774
0.311 -0.774 1.053
0.003 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.111 -0.202 0.246
-0.202 1.324 -1.392
0.246 -1.392 1.213
-0.009 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.093 -1.206 1.613
-1.206 -0.167 -1.699
1.613 -1.699 0.796
-0.009 -0.008 0.005
-0.011 -0.004 -0.005
0.003 0.005 -0.002

atensor 18 H
-1.804 -0.242 0.521
-0.242 -1.078 -1.733
0.521 -1.733 2.903
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.008 -0.004

atensor 19 C
0.507 0.431 -0.603
0.431 0.104 -0.391
-0.603 -0.391 0.455
0.002 0.001 -0.003
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.699 0.935 -0.820
0.935 -0.530 -0.868
-0.820 -0.868 -0.785
0.006 0.007 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.334 0.839 -2.146
0.838 -1.411 -1.090
-2.146 -1.090 1.159
0.002 0.000 -0.023
0.007 0.001 -0.015
-0.002 0.007 0.000

atensor 22 H
1.502 1.174 -1.475
1.174 -1.091 -0.598
-1.475 -0.598 -0.787
0.017 0.001 -0.012
0.010 0.001 -0.006
-0.005 0.001 0.000

atensor 23 C
0.784 0.575 0.454
0.575 0.176 0.276
0.454 0.276 0.108
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.104 -0.038 -0.018

-0.038 0.557 0.868
-0.018 0.868 0.962
0.004 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.152 0.143 0.074
0.143 1.614 1.362
0.074 1.362 0.962
-0.008 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.767 0.259 0.642
0.259 -0.673 2.114
0.642 2.114 2.460
-0.017 -0.009 0.010
-0.003 -0.001 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.801 -0.872 -1.135
-0.872 0.229 2.066
-1.135 2.066 1.108
-0.010 -0.010 -0.002
-0.010 -0.004 0.008
0.000 -0.003 -0.001

atensor 28 H
1.416 0.649 -0.224
0.649 0.551 -0.116
-0.224 -0.116 -0.034
0.008 0.002 -0.001
0.010 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
-0.068 0.351 -0.224
0.351 -2.465 -0.004
-0.224 -0.003 -1.650
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.113 1.886 0.348
1.886 0.446 0.669
0.348 0.669 0.734
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.040 1.396 0.588
1.396 -1.000 0.256
0.588 0.256 -1.417
0.020 0.002 0.007
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.774 1.338 2.100
1.338 -1.186 1.000
2.100 1.000 -0.172
0.008 0.001 0.021

0.010 0.002 0.012
-0.001 -0.008 -0.007

atensor 33 H
-0.335 1.191 0.568
1.191 -0.381 0.532
0.568 0.532 -1.297
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.548 2.877 -0.468
2.877 0.625 -0.612
-0.468 -0.612 -3.932
0.036 0.067 -0.006
0.014 -0.008 -0.001
-0.003 -0.007 0.016

atensor 35 H
0.210 -0.258 -0.107
-0.258 -0.732 0.033
-0.107 0.033 -0.720
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.360 -0.363 -0.056
-0.363 0.126 0.028
-0.056 0.028 -0.218
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.509 -0.625 -0.002
-0.625 0.506 0.012
-0.002 0.012 -0.785
-0.006 -0.005 0.001
-0.007 0.000 0.001
0.001 0.001 0.000

atensor 38 Cr
17.601 2.573 -0.264
2.573 26.950 -0.873
-0.264 -0.873 16.672
0.135 -0.805 0.320
-0.822 0.696 0.190
0.320 0.188 2.254

atensor 39 Br
31.683 1.582 10.767
1.582 11.957 -26.862
10.767 -26.862 -29.055
-1.251 -0.263 -0.514
-0.241 -0.149 2.582
-0.835 2.030 3.032

atensor 40 Br
22.422 5.827 -25.230
5.827 17.041 21.425
-25.230 21.425 -24.860
-0.633 -0.610 1.574
-0.695 -0.585 -2.105
1.897 -1.562 2.849

orbtensor 1 N
-479.333 53.189 47.189
53.189 -548.972 17.432
47.189 17.432 -95.265
338.750 -3.782 -2.113
-3.782 349.694 -1.043
-2.113 -1.043 320.986

orbtensor 2 C
-272.809 26.350 24.450
26.350 -297.960 8.582
24.450 8.582 -74.283
253.140 5.817 -5.648
5.817 251.785 -2.870
-5.648 -2.870 212.225

orbtensor 3 C
-219.895 -44.596 23.617
-44.596 -287.516 18.008
23.617 18.008 -57.452
252.431 3.307 -3.936
3.307 262.817 -2.517
-3.936 -2.517 223.635

orbtensor 4 C
-300.053 -23.695 32.688
-23.695 -232.997 12.439
32.688 12.439 -58.897
257.114 3.196 -5.255
3.196 253.215 -2.296
-5.255 -2.296 218.111

orbtensor 5 C
-287.857 2.875 29.647
2.875 -275.754 11.256
29.647 11.256 -59.098
269.113 0.365 -4.437
0.365 266.708 -1.738
-4.437 -1.738 235.207

orbtensor 6 C
-275.044 20.815 21.501
20.815 -296.206 7.749
21.501 7.749 -101.448
263.417 -5.183 -5.606
-5.183 261.096 -1.634
-5.606 -1.634 218.229

orbtensor 7 C
-296.781 10.290 30.102
10.290 -210.225 6.740
30.102 6.740 -61.200
258.100 -4.153 -4.984
-4.153 251.935 -1.285
-4.984 -1.285 218.097

orbtensor 8 C
-251.026 54.691 23.089
54.691 -268.125 4.587
23.089 4.587 -51.080
253.974 -5.686 -4.066
-5.686 255.806 -1.164
-4.066 -1.164 220.408

orbtensor 9 C
-234.354 -33.807 24.709
-33.807 -292.005 16.784

24.709	16.784	-59.002
253.150	-3.842	-4.172
-3.842	257.439	-1.533
-4.172	-1.533	219.543

orbtensor 10 C

-301.449	-15.850	28.358
-15.850	-249.921	10.636
28.358	10.636	-90.345
270.045	-1.183	-4.404
-1.183	264.970	-1.418
-4.404	-1.418	235.754

orbtensor 11 C

-219.922	31.186	-0.217
31.186	-131.627	-8.047
-0.217	-8.047	-208.332
248.019	-8.521	-1.124
-8.521	240.516	0.838
-1.124	0.838	235.823

orbtensor 12 C

-200.628	18.143	0.026
18.143	-105.442	24.269
0.026	24.269	-235.524
242.234	-2.874	-4.259
-2.874	236.428	-6.608
-4.259	-6.608	244.318

orbtensor 13 C

-227.692	-8.985	14.047
-8.985	-94.145	13.453
14.047	13.453	-220.105
245.616	4.710	-1.981
4.710	233.904	-4.384
-1.981	-4.384	244.418

orbtensor 14 C

-203.121	9.290	-9.134
9.290	-112.316	-40.723
-9.134	-40.723	-226.148
244.462	-0.585	4.218
-0.585	237.938	7.607
4.218	7.607	240.584

orbtensor 15 C

-57.332	0.543	6.355
0.543	-48.186	2.910
6.355	2.910	-50.683
219.030	-0.666	2.806
-0.666	218.693	-4.285
2.806	-4.285	228.230

orbtensor 16 H

3.192	-0.656	0.002
-0.656	1.940	1.387
0.002	1.387	1.457
23.260	0.390	-0.238
0.390	29.612	-6.893
-0.238	-6.893	29.170

orbtensor 17 H

3.294	0.444	-2.082
0.444	3.502	2.321
-2.082	2.321	2.843
30.083	-0.359	0.652
-0.359	21.044	-2.433

0.652	-2.433	28.631
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orbtensor 18 H

5.077	0.385	-0.146
0.385	3.246	2.179
-0.146	2.179	-1.283
21.126	-3.178	-0.400
-3.178	27.066	0.765
-0.400	0.765	30.090

orbtensor 19 C

-54.843	-0.471	-5.693
-0.471	-46.380	2.391
-5.693	2.391	-55.903
225.951	1.630	-6.830
1.630	219.190	-1.578
-6.830	-1.578	223.277

orbtensor 20 H

2.293	-0.623	1.098
-0.623	1.987	0.842
1.098	0.842	2.438
26.454	3.911	-3.980
3.911	29.332	-5.110
-3.980	-5.110	26.292

orbtensor 21 H

2.660	-1.614	2.721
-1.614	3.503	1.035
2.721	1.035	0.244
25.264	3.565	-3.063
3.565	25.439	2.708
-3.063	2.708	28.488

orbtensor 22 H

-0.917	-1.127	1.403
-1.127	2.954	1.218
1.403	1.218	3.693
33.480	-1.393	-0.791
-1.393	22.747	-1.384
-0.791	-1.384	25.652

orbtensor 23 C

-52.116	-0.634	4.839
-0.634	-46.984	-3.340
4.839	-3.340	-58.035
229.046	2.642	5.057
2.642	219.501	1.253
5.057	1.253	219.873

orbtensor 24 C

-59.997	-0.761	-3.842
-0.761	-48.812	-2.923
-3.842	-2.923	-47.400
218.235	0.394	-0.317
0.394	219.700	5.279
-0.317	5.279	228.018

orbtensor 25 H

3.106	-1.005	-0.306
-1.005	1.667	-1.194
-0.306	-1.194	1.814
23.694	2.181	1.340
2.181	31.010	6.354
1.340	6.354	27.338

orbtensor 26 H

4.752	-0.296	-1.364
-0.296	2.739	-2.609
-1.364	-2.609	-0.453
21.968	-3.057	2.856
-3.057	27.025	0.330
2.856	0.330	29.286

orbtensor 27 H

4.280	0.039	1.746
0.039	2.999	-2.454
1.746	-2.454	2.356
29.667	0.274	-0.988
0.274	21.638	3.202
-0.988	3.202	28.454

orbtensor 28 H

-5.449	-5.922	0.661
-5.922	-16.876	1.501
0.661	1.501	-2.879
32.070	4.818	-1.360
4.818	41.590	-1.572
-1.360	-1.572	23.668

orbtensor 29 H

-18.290	-3.039	2.292
-3.039	-3.599	0.493
2.292	0.493	-1.924
41.651	2.416	-2.732
2.416	30.576	-0.798
-2.732	-0.798	21.663

orbtensor 30 C

-233.681	-14.896	-8.798
-14.896	-98.004	-22.932
-8.798	-22.932	-210.238
246.347	5.936	0.790
5.936	234.785	3.988
0.790	3.988	242.791

orbtensor 31 H

-1.270	-1.455	0.056
-1.455	2.743	-0.759
0.056	-0.759	4.256
33.395	-0.985	-1.136
-0.985	23.102	1.950
-1.136	1.950	25.383

orbtensor 32 H

1.235	-2.148	-2.748
-2.148	3.303	-0.801
-2.748	-0.801	1.866
26.882	3.137	3.198
3.137	24.809	-3.262
3.198	-3.262	27.502

orbtensor 33 H

1.789	-0.908	-0.826
-0.908	1.837	-0.552
-0.826	-0.552	3.090
28.245	5.380	2.845
5.380	30.237	3.396
2.845	3.396	23.597

orbtensor 34 H

-8.513	4.270	0.722
4.270	-13.818	0.122
0.722	0.122	-1.208

35.528	-1.286	-1.907
-1.286	34.985	-0.619
-1.907	-0.619	20.363

orbtensor 35 H

-18.305	0.194	2.079
0.194	-3.345	0.048
2.079	0.048	-2.224
42.253	-0.368	-2.633
-0.368	30.338	-0.418
-2.633	-0.418	21.860

orbtensor 36 H

-8.516	7.871	0.264
7.871	-13.242	-0.478
0.264	-0.478	-3.218
34.452	-6.970	-1.067
-6.970	38.072	0.111
-1.067	0.111	23.368

orbtensor 37 H

-4.881	-4.747	0.679
-4.747	-16.705	1.405
0.679	1.405	-1.688
31.365	1.205	-1.286
1.205	40.413	-1.132
-1.286	-1.132	22.025

orbtensor 38 Cr

-5040.523	401.164	-78.879
401.164	-3571.210	-152.519
-78.879	-152.519	-5474.863
1810.105	-0.348	0.235
-0.348	1811.894	0.041
0.235	0.041	1811.770

orbtensor 39 Br

-872.955	-63.954	-2.676
-63.954	-1078.710	449.779
-2.676	449.779	-931.661
3090.062	-1.761	-3.348
-1.761	3096.688	8.392
-3.348	8.392	3099.539

orbtensor 40 Br

-870.735	-171.804	11.366
-171.804	-1167.968	-394.655
11.366	-394.655	-844.601
3092.386	-3.294	5.700
-3.294	3095.028	-7.374
5.700	-7.374	3098.875

gtensor (ppt)

-0.154	0.005	0.000
0.005	-0.156	-0.001
0.000	-0.001	-0.155
14.173	8.034	-1.802
8.034	13.646	-1.568
-1.802	-1.568	3.701

zfstensor (cm-1)

-9.250664	-0.809811	0.705660
-0.809811	-7.564635	0.281255
0.705660	0.281255	-4.178849

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.5657	-38.04667	4727.62462	-21.85487	4705.76975	4667.72308
2	C	3.5383	24.03267	-1873.88990	10.15014	-1863.73976	-1839.70709
3	C	-0.6670	58.00667	353.24104	-7.56384	345.67720	403.68387
4	C	1.2263	45.49767	-649.46217	14.84068	-634.62149	-589.12382
5	C	-1.1093	49.43967	587.49935	-3.21711	584.28224	633.72191
6	C	0.5177	23.34800	-274.15459	1.03479	-273.11981	-249.77181
7	C	0.2357	53.30867	-124.80831	2.88479	-121.92351	-68.61485
8	C	-0.3597	53.31900	190.47830	-1.64914	188.82917	242.14817
9	C	-0.7720	48.25700	408.84871	4.09845	412.94715	461.20415
10	C	0.6347	43.01800	-336.11742	-2.89083	-339.00825	-295.99025
11	C	-0.4747	54.82567	251.38193	5.28589	256.66782	311.49349
12	C	1.3117	60.46200	-694.65443	2.28373	-692.37069	-631.90869
13	C	1.1397	60.66533	-603.56378	-7.80137	-611.36515	-550.69982
14	C	1.3117	60.46633	-694.65443	2.22979	-692.42464	-631.95830
15	C	0.4753	169.91733	-251.73500	3.99296	-247.74203	-77.82470
16	H	0.8073	29.54367	-107.53326	0.82376	-106.70950	-77.16583
17	H	0.1737	29.79900	-23.13164	2.09182	-21.03981	8.75919
18	H	-0.0003	28.44067	0.04440	4.02050	4.06489	32.50556
19	C	0.3597	170.43067	-190.47830	-2.54715	-193.02545	-22.59478
20	H	-0.6677	29.59867	88.93027	-1.39679	87.53348	117.13215
21	H	-0.1943	28.53267	25.88435	-0.30744	25.57691	54.10958
22	H	-0.1193	29.20300	15.89468	-3.15699	12.73768	41.94068
23	C	0.3603	170.42833	-190.83137	-2.55713	-193.38850	-22.96017
24	C	0.4747	169.91467	-251.38193	3.97359	-247.40835	-77.49368
25	H	0.8067	29.54300	-107.44446	0.81656	-106.62790	-77.08490
26	H	-0.0013	28.43900	0.17759	4.01096	4.18855	32.62755
27	H	0.1737	29.79800	-23.13164	2.07930	-21.05234	8.74566
28	H	0.6493	24.04133	-86.48835	-1.71946	-88.20781	-64.16648
29	H	-1.3933	23.35900	185.58589	-1.24419	184.34170	207.70070
30	C	1.1387	60.66667	-603.03419	-7.82027	-610.85445	-550.18779
31	H	-0.1193	29.20300	15.89468	-3.15862	12.73606	41.93906
32	H	-0.1937	28.53233	25.79555	-0.31229	25.48326	54.01559
33	H	-0.6673	29.59833	88.88587	-1.40073	87.48515	117.08348
34	H	-1.6037	22.44567	213.60137	-5.15997	208.44140	230.88707
35	H	-0.4133	23.52567	55.05419	-0.45137	54.60282	78.12848
36	H	0.0890	23.63867	-11.85441	-0.19101	-12.04542	11.59324
37	H	-0.2647	23.50967	35.25244	0.03666	35.28910	58.79877
38	Cr	21.4360	-2884.27567	50411.46315	45.31572	50456.77887	47572.50321
39	Br	5.4057	2134.32100	-2863.95900	-187.75787	-3051.71686	-917.39586
40	Br	5.4113	2134.32833	-2866.96124	-188.41193	-3055.37316	-921.04483

=====
CrL2-STO-BP-Pederson
Temperature: 298
Spin: 1.5

atensor 1 N
-1.780 0.249 -0.227
0.249 -2.529 -0.081
-0.227 -0.081 -3.422
0.003 0.014 0.001
0.002 0.012 0.000
0.002 -0.001 0.019

atensor 2 C
2.656 0.978 0.387
0.978 1.915 0.094
0.387 0.094 6.033
-0.059 -0.015 0.009
0.077 0.064 -0.013
0.004 -0.001 0.006

atensor 3 C
0.205 0.180 -0.270

0.180 -0.412 -0.098
-0.270 -0.098 -1.797
0.005 -0.004 0.000
0.006 -0.002 -0.001
-0.001 0.001 0.000

atensor 4 C
0.121 0.097 0.503
0.097 -0.444 0.227
0.503 0.227 4.022
0.002 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.613 -0.080 -0.130
-0.080 -1.074 -0.021
-0.130 -0.021 -1.649
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.056
-0.446 -0.676 0.135
-0.056 0.135 0.811
0.014 -0.011 -0.002
-0.016 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.123 -0.100 0.086
-0.100 -0.149 0.060
0.086 0.060 0.738
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.132 -0.152 -0.069
-0.152 -0.225 -0.007
-0.069 -0.007 -0.725
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.103 -0.248 0.129
-0.248 -0.986 0.073
0.129 0.073 -0.214
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.336 -0.947 -0.170
-0.947 0.942 0.051
-0.170 0.051 -0.368
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.386 -1.501 0.022
-1.501 -1.847 0.286
0.022 0.286 -0.077
0.044 0.002 0.002

0.000 0.010 0.003
0.002 0.002 0.060

atensor 12 C
0.250 -0.484 0.080
-0.484 2.179 -2.299
0.080 -2.299 1.440
0.012 0.013 -0.014
-0.032 0.011 -0.027
-0.006 0.013 0.043

atensor 13 C
1.814 1.602 -0.794
1.602 0.264 -1.054
-0.794 -1.054 1.218
0.023 0.020 -0.008
-0.023 0.028 0.026
0.007 0.003 0.072

atensor 14 C
0.284 0.102 0.179
0.102 2.656 2.220
0.179 2.220 0.929
0.019 0.011 0.018
-0.023 0.013 0.037
0.015 -0.013 0.034

atensor 15 C
-0.021 -0.231 0.311
-0.231 0.385 -0.774
0.311 -0.774 1.053
0.003 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.111 -0.202 0.246
-0.202 1.324 -1.392
0.246 -1.392 1.213
-0.009 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.093 -1.206 1.613
-1.206 -0.167 -1.699
1.613 -1.699 0.796
-0.009 -0.008 0.005
-0.011 -0.004 -0.005
0.003 0.005 -0.002

atensor 18 H
-1.804 -0.242 0.521
-0.242 -1.078 -1.733
0.521 -1.733 2.903
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.008 -0.004

atensor 19 C
0.507 0.431 -0.603
0.431 0.104 -0.391
-0.603 -0.391 0.455
0.002 0.001 -0.003
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.699 0.935 -0.820
0.935 -0.530 -0.868
-0.820 -0.868 -0.785
0.006 0.007 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.334 0.839 -2.146
0.838 -1.411 -1.090
-2.146 -1.090 1.159
0.002 0.000 -0.023
0.007 0.001 -0.015
-0.002 0.007 0.000

atensor 22 H
1.502 1.174 -1.475
1.174 -1.091 -0.598
-1.475 -0.598 -0.787
0.017 0.001 -0.012
0.010 0.001 -0.006
-0.005 0.001 0.000

atensor 23 C
0.784 0.575 0.454
0.575 0.176 0.276
0.454 0.276 0.108
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.104 -0.038 -0.018
-0.038 0.557 0.868
-0.018 0.868 0.962
0.004 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.152 0.143 0.074
0.143 1.614 1.362
0.074 1.362 0.962
-0.008 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.767 0.259 0.642
0.259 -0.673 2.114
0.642 2.114 2.460
-0.017 -0.009 0.010
-0.003 -0.001 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.801 -0.872 -1.135
-0.872 0.229 2.066
-1.135 2.066 1.108
-0.010 -0.010 -0.002
-0.010 -0.004 0.008
0.000 -0.003 -0.001

atensor 28 H
1.416 0.649 -0.224
0.649 0.551 -0.116

-0.224 -0.116 -0.034
0.008 0.002 -0.001
0.010 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
-0.068 0.351 -0.224
0.351 -2.465 -0.004
-0.224 -0.003 -1.650
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.113 1.886 0.348
1.886 0.446 0.669
0.348 0.669 0.734
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.040 1.396 0.588
1.396 -1.000 0.256
0.588 0.256 -1.417
0.020 0.002 0.007
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.774 1.338 2.100
1.338 -1.186 1.000
2.100 1.000 -0.172
0.008 0.001 0.021
0.010 0.002 0.012
-0.001 -0.008 -0.007

atensor 33 H
-0.335 1.191 0.568
1.191 -0.381 0.532
0.568 0.532 -1.297
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.548 2.877 -0.468
2.877 0.625 -0.612
-0.468 -0.612 -3.932
0.036 0.067 -0.006
0.014 -0.008 -0.001
-0.003 -0.007 0.016

atensor 35 H
0.210 -0.258 -0.107
-0.258 -0.732 0.033
-0.107 0.033 -0.720
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.360 -0.363 -0.056
-0.363 0.126 0.028
-0.056 0.028 -0.218
0.000 -0.002 0.000
-0.002 -0.001 0.000

0.000 0.000 0.000

atensor 37 H

-0.509 -0.625 -0.002
-0.625 0.506 0.012
-0.002 0.012 -0.785
-0.006 -0.005 0.001
-0.007 0.000 0.001
0.001 0.001 0.000

atensor 38 Cr

17.601 2.573 -0.264
2.573 26.950 -0.873
-0.264 -0.873 16.672
0.135 -0.805 0.320
-0.822 0.696 0.190
0.320 0.188 2.254

atensor 39 Br

31.683 1.582 10.767
1.582 11.957 -26.862
10.767 -26.862 -29.055
-1.251 -0.263 -0.514
-0.241 -0.149 2.582
-0.835 2.030 3.032

atensor 40 Br

22.422 5.827 -25.230
5.827 17.041 21.425
-25.230 21.425 -24.860
-0.633 -0.610 1.574
-0.695 -0.585 -2.105
1.897 -1.562 2.849

orbtensor 1 N

-479.333 53.189 47.189
53.189 -548.972 17.432
47.189 17.432 -95.265
338.750 -3.782 -2.113
-3.782 349.694 -1.043
-2.113 -1.043 320.986

orbtensor 2 C

-272.809 26.350 24.450
26.350 -297.960 8.582
24.450 8.582 -74.283
253.140 5.817 -5.648
5.817 251.785 -2.870
-5.648 -2.870 212.225

orbtensor 3 C

-219.895 -44.596 23.617
-44.596 -287.516 18.008
23.617 18.008 -57.452
252.431 3.307 -3.936
3.307 262.817 -2.517
-3.936 -2.517 223.635

orbtensor 4 C

-300.053 -23.695 32.688
-23.695 -232.997 12.439
32.688 12.439 -58.897
257.114 3.196 -5.255
3.196 253.215 -2.296
-5.255 -2.296 218.111

orbtensor 5 C

-287.857	2.875	29.647
2.875	-275.754	11.256
29.647	11.256	-59.098
269.113	0.365	-4.437
0.365	266.708	-1.738
-4.437	-1.738	235.207

orbtensor 6 C

-275.044	20.815	21.501
20.815	-296.206	7.749
21.501	7.749	-101.448
263.417	-5.183	-5.606
-5.183	261.096	-1.634
-5.606	-1.634	218.229

orbtensor 7 C

-296.781	10.290	30.102
10.290	-210.225	6.740
30.102	6.740	-61.200
258.100	-4.153	-4.984
-4.153	251.935	-1.285
-4.984	-1.285	218.097

orbtensor 8 C

-251.026	54.691	23.089
54.691	-268.125	4.587
23.089	4.587	-51.080
253.974	-5.686	-4.066
-5.686	255.806	-1.164
-4.066	-1.164	220.408

orbtensor 9 C

-234.354	-33.807	24.709
-33.807	-292.005	16.784
24.709	16.784	-59.002
253.150	-3.842	-4.172
-3.842	257.439	-1.533
-4.172	-1.533	219.543

orbtensor 10 C

-301.449	-15.850	28.358
-15.850	-249.921	10.636
28.358	10.636	-90.345
270.045	-1.183	-4.404
-1.183	264.970	-1.418
-4.404	-1.418	235.754

orbtensor 11 C

-219.922	31.186	-0.217
31.186	-131.627	-8.047
-0.217	-8.047	-208.332
248.019	-8.521	-1.124
-8.521	240.516	0.838
-1.124	0.838	235.823

orbtensor 12 C

-200.628	18.143	0.026
18.143	-105.442	24.269
0.026	24.269	-235.524
242.234	-2.874	-4.259
-2.874	236.428	-6.608
-4.259	-6.608	244.318

orbtensor 13 C

-227.692	-8.985	14.047
-8.985	-94.145	13.453
14.047	13.453	-220.105

245.616	4.710	-1.981
4.710	233.904	-4.384
-1.981	-4.384	244.418

orbtensor 14 C

-203.121	9.290	-9.134
9.290	-112.316	-40.723
-9.134	-40.723	-226.148
244.462	-0.585	4.218
-0.585	237.938	7.607
4.218	7.607	240.584

orbtensor 15 C

-57.332	0.543	6.355
0.543	-48.186	2.910
6.355	2.910	-50.683
219.030	-0.666	2.806
-0.666	218.693	-4.285
2.806	-4.285	228.230

orbtensor 16 H

3.192	-0.656	0.002
-0.656	1.940	1.387
0.002	1.387	1.457
23.260	0.390	-0.238
0.390	29.612	-6.893
-0.238	-6.893	29.170

orbtensor 17 H

3.294	0.444	-2.082
0.444	3.502	2.321
-2.082	2.321	2.843
30.083	-0.359	0.652
-0.359	21.044	-2.433
0.652	-2.433	28.631

orbtensor 18 H

5.077	0.385	-0.146
0.385	3.246	2.179
-0.146	2.179	-1.283
21.126	-3.178	-0.400
-3.178	27.066	0.765
-0.400	0.765	30.090

orbtensor 19 C

-54.843	-0.471	-5.693
-0.471	-46.380	2.391
-5.693	2.391	-55.903
225.951	1.630	-6.830
1.630	219.190	-1.578
-6.830	-1.578	223.277

orbtensor 20 H

2.293	-0.623	1.098
-0.623	1.987	0.842
1.098	0.842	2.438
26.454	3.911	-3.980
3.911	29.332	-5.110
-3.980	-5.110	26.292

orbtensor 21 H

2.660	-1.614	2.721
-1.614	3.503	1.035
2.721	1.035	0.244
25.264	3.565	-3.063
3.565	25.439	2.708
-3.063	2.708	28.488

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orbtensor 22 H
-0.917   -1.127    1.403
-1.127    2.954    1.218
 1.403    1.218    3.693
33.480   -1.393   -0.791
-1.393   22.747   -1.384
-0.791   -1.384   25.652

orbtensor 23 C
-52.116   -0.634    4.839
-0.634  -46.984   -3.340
 4.839   -3.340  -58.035
229.046    2.642    5.057
 2.642  219.501    1.253
 5.057    1.253  219.873

orbtensor 24 C
-59.997   -0.761   -3.842
-0.761  -48.812   -2.923
-3.842  -2.923  -47.400
218.235    0.394   -0.317
 0.394  219.700    5.279
-0.317    5.279  228.018

orbtensor 25 H
 3.106   -1.005   -0.306
-1.005    1.667   -1.194
-0.306   -1.194    1.814
23.694    2.181    1.340
 2.181   31.010    6.354
 1.340    6.354   27.338

orbtensor 26 H
 4.752   -0.296   -1.364
-0.296    2.739   -2.609
-1.364   -2.609   -0.453
21.968   -3.057    2.856
-3.057   27.025    0.330
 2.856    0.330   29.286

orbtensor 27 H
 4.280    0.039    1.746
 0.039    2.999   -2.454
 1.746   -2.454    2.356
29.667    0.274   -0.988
 0.274   21.638    3.202
-0.988    3.202   28.454

orbtensor 28 H
-5.449   -5.922    0.661
-5.922  -16.876    1.501
 0.661    1.501   -2.879
32.070    4.818   -1.360
 4.818   41.590   -1.572
-1.360   -1.572   23.668

orbtensor 29 H
-18.290   -3.039    2.292
-3.039   -3.599    0.493
 2.292    0.493   -1.924
41.651    2.416   -2.732
 2.416   30.576   -0.798
-2.732   -0.798   21.663

orbtensor 30 C
-233.681  -14.896   -8.798

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-14.896	-98.004	-22.932
-8.798	-22.932	-210.238
246.347	5.936	0.790
5.936	234.785	3.988
0.790	3.988	242.791

orbtensor 31 H

-1.270	-1.455	0.056
-1.455	2.743	-0.759
0.056	-0.759	4.256
33.395	-0.985	-1.136
-0.985	23.102	1.950
-1.136	1.950	25.383

orbtensor 32 H

1.235	-2.148	-2.748
-2.148	3.303	-0.801
-2.748	-0.801	1.866
26.882	3.137	3.198
3.137	24.809	-3.262
3.198	-3.262	27.502

orbtensor 33 H

1.789	-0.908	-0.826
-0.908	1.837	-0.552
-0.826	-0.552	3.090
28.245	5.380	2.845
5.380	30.237	3.396
2.845	3.396	23.597

orbtensor 34 H

-8.513	4.270	0.722
4.270	-13.818	0.122
0.722	0.122	-1.208
35.528	-1.286	-1.907
-1.286	34.985	-0.619
-1.907	-0.619	20.363

orbtensor 35 H

-18.305	0.194	2.079
0.194	-3.345	0.048
2.079	0.048	-2.224
42.253	-0.368	-2.633
-0.368	30.338	-0.418
-2.633	-0.418	21.860

orbtensor 36 H

-8.516	7.871	0.264
7.871	-13.242	-0.478
0.264	-0.478	-3.218
34.452	-6.970	-1.067
-6.970	38.072	0.111
-1.067	0.111	23.368

orbtensor 37 H

-4.881	-4.747	0.679
-4.747	-16.705	1.405
0.679	1.405	-1.688
31.365	1.205	-1.286
1.205	40.413	-1.132
-1.286	-1.132	22.025

orbtensor 38 Cr

-5040.523	401.164	-78.879
401.164	-3571.210	-152.519
-78.879	-152.519	-5474.863
1810.105	-0.348	0.235

-0.348 1811.894 0.041
 0.235 0.041 1811.770

orbtensor 39 Br
 -872.955 -63.954 -2.676
 -63.954 -1078.710 449.779
 -2.676 449.779 -931.661
 3090.062 -1.761 -3.348
 -1.761 3096.688 8.392
 -3.348 8.392 3099.539

orbtensor 40 Br
 -870.735 -171.804 11.366
 -171.804 -1167.968 -394.655
 11.366 -394.655 -844.601
 3092.386 -3.294 5.700
 -3.294 3095.028 -7.374
 5.700 -7.374 3098.875

gtensor (ppt)
 -0.154 0.005 0.000
 0.005 -0.156 -0.001
 0.000 -0.001 -0.155
 14.173 8.034 -1.802
 8.034 13.646 -1.568
 -1.802 -1.568 3.701

zfstensor (cm-1)
 -0.372341 0.368525 0.131492
 0.368525 -0.111407 -0.079684
 0.131492 -0.079684 0.483748

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.5657	-38.04667	4727.41434	-6.24432	4721.17002	4683.12335
2	C	3.5383	24.03267	-1873.80655	3.56738	-1870.23917	-1846.20650
3	C	-0.6670	58.00667	353.22533	-2.23311	350.99222	408.99889
4	C	1.2263	45.49767	-649.43328	4.73323	-644.70006	-599.20239
5	C	-1.1093	49.43967	587.47322	-0.97899	586.49423	635.93389
6	C	0.5177	23.34800	-274.14240	0.42015	-273.72225	-250.37425
7	C	0.2357	53.30867	-124.80275	0.90043	-123.90232	-70.59366
8	C	-0.3597	53.31900	190.46983	-0.55359	189.91624	243.23524
9	C	-0.7720	48.25700	408.83052	1.18332	410.01384	458.27084
10	C	0.6347	43.01800	-336.10247	-1.16595	-337.26842	-294.25042
11	C	-0.4747	54.82567	251.37075	1.42430	252.79505	307.62072
12	C	1.3117	60.46200	-694.62353	0.68900	-693.93453	-633.47253
13	C	1.1397	60.66533	-603.53694	-1.62922	-605.16616	-544.50082
14	C	1.3117	60.46633	-694.62353	0.10321	-694.52032	-634.05399
15	C	0.4753	169.91733	-251.72380	1.25992	-250.46388	-80.54655
16	H	0.8073	29.54367	-107.52848	0.25464	-107.27384	-77.73017
17	H	0.1737	29.79900	-23.13061	0.64276	-22.48785	7.31115
18	H	-0.0003	28.44067	0.04440	1.29012	1.33451	29.77518
19	C	0.3597	170.43067	-190.46983	-0.57611	-191.04594	-20.61527
20	H	-0.6677	29.59867	88.92632	-0.34270	88.58362	118.18229
21	H	-0.1943	28.53267	25.88320	0.02669	25.90989	54.44255
22	H	-0.1193	29.20300	15.89397	-0.80733	15.08664	44.28964
23	C	0.3603	170.42833	-190.82288	-0.57820	-191.40108	-20.97275
24	C	0.4747	169.91467	-251.37075	1.01888	-250.35187	-80.43720
25	H	0.8067	29.54300	-107.43968	0.16039	-107.27930	-77.73630
26	H	-0.0013	28.43900	0.17759	1.16597	1.34356	29.78256
27	H	0.1737	29.79800	-23.13061	0.46191	-22.66870	7.12930
28	H	0.6493	24.04133	-86.48451	-0.45898	-86.94348	-62.90215
29	H	-1.3933	23.35900	185.57764	-0.29121	185.28643	208.64543
30	C	1.1387	60.66667	-603.00736	-1.75869	-604.76605	-544.09939
31	H	-0.1193	29.20300	15.89397	-0.79317	15.10080	44.30380

32	H	-0.1937	28.53233	25.79440	0.04466	25.83906	54.37140
33	H	-0.6673	29.59833	88.88192	-0.36045	88.52147	118.11980
34	H	-1.6037	22.44567	213.59187	-1.43556	212.15631	234.60197
35	H	-0.4133	23.52567	55.05174	-0.13496	54.91678	78.44244
36	H	0.0890	23.63867	-11.85388	-0.08261	-11.93650	11.70217
37	H	-0.2647	23.50967	35.25087	-0.06912	35.18175	58.69142
38	Cr	21.4360	-2884.27567	50409.22086	16.64162	50425.86248	47541.58681
39	Br	5.4057	2134.32100	-2863.83161	-52.05647	-2915.88808	-781.56708
40	Br	5.4113	2134.32833	-2866.83371	-60.61224	-2927.44595	-793.11762

=====
 CrL2-STO-BP-Van-Wullen

Temperature: 298

Spin: 1.5

atensor 1 N

-1.780 0.249 -0.227
 0.249 -2.529 -0.081
 -0.227 -0.081 -3.422
 0.003 0.014 0.001
 0.002 0.012 0.000
 0.002 -0.001 0.019

atensor 2 C

2.656 0.978 0.387
 0.978 1.915 0.094
 0.387 0.094 6.033
 -0.059 -0.015 0.009
 0.077 0.064 -0.013
 0.004 -0.001 0.006

atensor 3 C

0.205 0.180 -0.270
 0.180 -0.412 -0.098
 -0.270 -0.098 -1.797
 0.005 -0.004 0.000
 0.006 -0.002 -0.001
 -0.001 0.001 0.000

atensor 4 C

0.121 0.097 0.503
 0.097 -0.444 0.227
 0.503 0.227 4.022
 0.002 0.010 -0.001
 -0.015 -0.021 0.003
 0.000 0.000 -0.001

atensor 5 C

-0.613 -0.080 -0.130
 -0.080 -1.074 -0.021
 -0.130 -0.021 -1.649
 0.003 -0.003 0.000
 0.000 0.005 0.000
 0.000 0.000 0.000

atensor 6 C

1.436 -0.446 -0.056
 -0.446 -0.676 0.135
 -0.056 0.135 0.811
 0.014 -0.011 -0.002
 -0.016 -0.029 0.003
 -0.001 0.003 -0.003

atensor 7 C

0.123 -0.100 0.086
 -0.100 -0.149 0.060

0.086 0.060 0.738
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.132 -0.152 -0.069
-0.152 -0.225 -0.007
-0.069 -0.007 -0.725
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.103 -0.248 0.129
-0.248 -0.986 0.073
0.129 0.073 -0.214
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.336 -0.947 -0.170
-0.947 0.942 0.051
-0.170 0.051 -0.368
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.386 -1.501 0.022
-1.501 -1.847 0.286
0.022 0.286 -0.077
0.044 0.002 0.002
0.000 0.010 0.003
0.002 0.002 0.060

atensor 12 C
0.250 -0.484 0.080
-0.484 2.179 -2.299
0.080 -2.299 1.440
0.012 0.013 -0.014
-0.032 0.011 -0.027
-0.006 0.013 0.043

atensor 13 C
1.814 1.602 -0.794
1.602 0.264 -1.054
-0.794 -1.054 1.218
0.023 0.020 -0.008
-0.023 0.028 0.026
0.007 0.003 0.072

atensor 14 C
0.284 0.102 0.179
0.102 2.656 2.220
0.179 2.220 0.929
0.019 0.011 0.018
-0.023 0.013 0.037
0.015 -0.013 0.034

atensor 15 C
-0.021 -0.231 0.311
-0.231 0.385 -0.774
0.311 -0.774 1.053
0.003 0.000 -0.005
-0.004 0.003 -0.002

0.001 0.007 0.003

atensor 16 H
-0.111 -0.202 0.246
-0.202 1.324 -1.392
0.246 -1.392 1.213
-0.009 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.093 -1.206 1.613
-1.206 -0.167 -1.699
1.613 -1.699 0.796
-0.009 -0.008 0.005
-0.011 -0.004 -0.005
0.003 0.005 -0.002

atensor 18 H
-1.804 -0.242 0.521
-0.242 -1.078 -1.733
0.521 -1.733 2.903
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.008 -0.004

atensor 19 C
0.507 0.431 -0.603
0.431 0.104 -0.391
-0.603 -0.391 0.455
0.002 0.001 -0.003
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.699 0.935 -0.820
0.935 -0.530 -0.868
-0.820 -0.868 -0.785
0.006 0.007 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.334 0.839 -2.146
0.838 -1.411 -1.090
-2.146 -1.090 1.159
0.002 0.000 -0.023
0.007 0.001 -0.015
-0.002 0.007 0.000

atensor 22 H
1.502 1.174 -1.475
1.174 -1.091 -0.598
-1.475 -0.598 -0.787
0.017 0.001 -0.012
0.010 0.001 -0.006
-0.005 0.001 0.000

atensor 23 C
0.784 0.575 0.454
0.575 0.176 0.276
0.454 0.276 0.108
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C

-0.104 -0.038 -0.018
-0.038 0.557 0.868
-0.018 0.868 0.962
0.004 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.152 0.143 0.074
0.143 1.614 1.362
0.074 1.362 0.962
-0.008 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.767 0.259 0.642
0.259 -0.673 2.114
0.642 2.114 2.460
-0.017 -0.009 0.010
-0.003 -0.001 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.801 -0.872 -1.135
-0.872 0.229 2.066
-1.135 2.066 1.108
-0.010 -0.010 -0.002
-0.010 -0.004 0.008
0.000 -0.003 -0.001

atensor 28 H
1.416 0.649 -0.224
0.649 0.551 -0.116
-0.224 -0.116 -0.034
0.008 0.002 -0.001
0.010 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
-0.068 0.351 -0.224
0.351 -2.465 -0.004
-0.224 -0.003 -1.650
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.113 1.886 0.348
1.886 0.446 0.669
0.348 0.669 0.734
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.040 1.396 0.588
1.396 -1.000 0.256
0.588 0.256 -1.417
0.020 0.002 0.007
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.774 1.338 2.100
1.338 -1.186 1.000
2.100 1.000 -0.172

0.008 0.001 0.021
0.010 0.002 0.012
-0.001 -0.008 -0.007

atensor 33 H
-0.335 1.191 0.568
1.191 -0.381 0.532
0.568 0.532 -1.297
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.548 2.877 -0.468
2.877 0.625 -0.612
-0.468 -0.612 -3.932
0.036 0.067 -0.006
0.014 -0.008 -0.001
-0.003 -0.007 0.016

atensor 35 H
0.210 -0.258 -0.107
-0.258 -0.732 0.033
-0.107 0.033 -0.720
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.360 -0.363 -0.056
-0.363 0.126 0.028
-0.056 0.028 -0.218
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.509 -0.625 -0.002
-0.625 0.506 0.012
-0.002 0.012 -0.785
-0.006 -0.005 0.001
-0.007 0.000 0.001
0.001 0.001 0.000

atensor 38 Cr
17.601 2.573 -0.264
2.573 26.950 -0.873
-0.264 -0.873 16.672
0.135 -0.805 0.320
-0.822 0.696 0.190
0.320 0.188 2.254

atensor 39 Br
31.683 1.582 10.767
1.582 11.957 -26.862
10.767 -26.862 -29.055
-1.251 -0.263 -0.514
-0.241 -0.149 2.582
-0.835 2.030 3.032

atensor 40 Br
22.422 5.827 -25.230
5.827 17.041 21.425
-25.230 21.425 -24.860
-0.633 -0.610 1.574
-0.695 -0.585 -2.105
1.897 -1.562 2.849

orbtensor 1 N
-479.333 53.189 47.189
53.189 -548.972 17.432
47.189 17.432 -95.265
338.750 -3.782 -2.113
-3.782 349.694 -1.043
-2.113 -1.043 320.986

orbtensor 2 C
-272.809 26.350 24.450
26.350 -297.960 8.582
24.450 8.582 -74.283
253.140 5.817 -5.648
5.817 251.785 -2.870
-5.648 -2.870 212.225

orbtensor 3 C
-219.895 -44.596 23.617
-44.596 -287.516 18.008
23.617 18.008 -57.452
252.431 3.307 -3.936
3.307 262.817 -2.517
-3.936 -2.517 223.635

orbtensor 4 C
-300.053 -23.695 32.688
-23.695 -232.997 12.439
32.688 12.439 -58.897
257.114 3.196 -5.255
3.196 253.215 -2.296
-5.255 -2.296 218.111

orbtensor 5 C
-287.857 2.875 29.647
2.875 -275.754 11.256
29.647 11.256 -59.098
269.113 0.365 -4.437
0.365 266.708 -1.738
-4.437 -1.738 235.207

orbtensor 6 C
-275.044 20.815 21.501
20.815 -296.206 7.749
21.501 7.749 -101.448
263.417 -5.183 -5.606
-5.183 261.096 -1.634
-5.606 -1.634 218.229

orbtensor 7 C
-296.781 10.290 30.102
10.290 -210.225 6.740
30.102 6.740 -61.200
258.100 -4.153 -4.984
-4.153 251.935 -1.285
-4.984 -1.285 218.097

orbtensor 8 C
-251.026 54.691 23.089
54.691 -268.125 4.587
23.089 4.587 -51.080
253.974 -5.686 -4.066
-5.686 255.806 -1.164
-4.066 -1.164 220.408

orbtensor 9 C
-234.354 -33.807 24.709

-33.807	-292.005	16.784
24.709	16.784	-59.002
253.150	-3.842	-4.172
-3.842	257.439	-1.533
-4.172	-1.533	219.543

orbtensor 10 C

-301.449	-15.850	28.358
-15.850	-249.921	10.636
28.358	10.636	-90.345
270.045	-1.183	-4.404
-1.183	264.970	-1.418
-4.404	-1.418	235.754

orbtensor 11 C

-219.922	31.186	-0.217
31.186	-131.627	-8.047
-0.217	-8.047	-208.332
248.019	-8.521	-1.124
-8.521	240.516	0.838
-1.124	0.838	235.823

orbtensor 12 C

-200.628	18.143	0.026
18.143	-105.442	24.269
0.026	24.269	-235.524
242.234	-2.874	-4.259
-2.874	236.428	-6.608
-4.259	-6.608	244.318

orbtensor 13 C

-227.692	-8.985	14.047
-8.985	-94.145	13.453
14.047	13.453	-220.105
245.616	4.710	-1.981
4.710	233.904	-4.384
-1.981	-4.384	244.418

orbtensor 14 C

-203.121	9.290	-9.134
9.290	-112.316	-40.723
-9.134	-40.723	-226.148
244.462	-0.585	4.218
-0.585	237.938	7.607
4.218	7.607	240.584

orbtensor 15 C

-57.332	0.543	6.355
0.543	-48.186	2.910
6.355	2.910	-50.683
219.030	-0.666	2.806
-0.666	218.693	-4.285
2.806	-4.285	228.230

orbtensor 16 H

3.192	-0.656	0.002
-0.656	1.940	1.387
0.002	1.387	1.457
23.260	0.390	-0.238
0.390	29.612	-6.893
-0.238	-6.893	29.170

orbtensor 17 H

3.294	0.444	-2.082
0.444	3.502	2.321
-2.082	2.321	2.843
30.083	-0.359	0.652

-0.359	21.044	-2.433
0.652	-2.433	28.631

orbtensor 18 H

5.077	0.385	-0.146
0.385	3.246	2.179
-0.146	2.179	-1.283
21.126	-3.178	-0.400
-3.178	27.066	0.765
-0.400	0.765	30.090

orbtensor 19 C

-54.843	-0.471	-5.693
-0.471	-46.380	2.391
-5.693	2.391	-55.903
225.951	1.630	-6.830
1.630	219.190	-1.578
-6.830	-1.578	223.277

orbtensor 20 H

2.293	-0.623	1.098
-0.623	1.987	0.842
1.098	0.842	2.438
26.454	3.911	-3.980
3.911	29.332	-5.110
-3.980	-5.110	26.292

orbtensor 21 H

2.660	-1.614	2.721
-1.614	3.503	1.035
2.721	1.035	0.244
25.264	3.565	-3.063
3.565	25.439	2.708
-3.063	2.708	28.488

orbtensor 22 H

-0.917	-1.127	1.403
-1.127	2.954	1.218
1.403	1.218	3.693
33.480	-1.393	-0.791
-1.393	22.747	-1.384
-0.791	-1.384	25.652

orbtensor 23 C

-52.116	-0.634	4.839
-0.634	-46.984	-3.340
4.839	-3.340	-58.035
229.046	2.642	5.057
2.642	219.501	1.253
5.057	1.253	219.873

orbtensor 24 C

-59.997	-0.761	-3.842
-0.761	-48.812	-2.923
-3.842	-2.923	-47.400
218.235	0.394	-0.317
0.394	219.700	5.279
-0.317	5.279	228.018

orbtensor 25 H

3.106	-1.005	-0.306
-1.005	1.667	-1.194
-0.306	-1.194	1.814
23.694	2.181	1.340
2.181	31.010	6.354
1.340	6.354	27.338

orbtensor 26 H
4.752 -0.296 -1.364
-0.296 2.739 -2.609
-1.364 -2.609 -0.453
21.968 -3.057 2.856
-3.057 27.025 0.330
2.856 0.330 29.286

orbtensor 27 H
4.280 0.039 1.746
0.039 2.999 -2.454
1.746 -2.454 2.356
29.667 0.274 -0.988
0.274 21.638 3.202
-0.988 3.202 28.454

orbtensor 28 H
-5.449 -5.922 0.661
-5.922 -16.876 1.501
0.661 1.501 -2.879
32.070 4.818 -1.360
4.818 41.590 -1.572
-1.360 -1.572 23.668

orbtensor 29 H
-18.290 -3.039 2.292
-3.039 -3.599 0.493
2.292 0.493 -1.924
41.651 2.416 -2.732
2.416 30.576 -0.798
-2.732 -0.798 21.663

orbtensor 30 C
-233.681 -14.896 -8.798
-14.896 -98.004 -22.932
-8.798 -22.932 -210.238
246.347 5.936 0.790
5.936 234.785 3.988
0.790 3.988 242.791

orbtensor 31 H
-1.270 -1.455 0.056
-1.455 2.743 -0.759
0.056 -0.759 4.256
33.395 -0.985 -1.136
-0.985 23.102 1.950
-1.136 1.950 25.383

orbtensor 32 H
1.235 -2.148 -2.748
-2.148 3.303 -0.801
-2.748 -0.801 1.866
26.882 3.137 3.198
3.137 24.809 -3.262
3.198 -3.262 27.502

orbtensor 33 H
1.789 -0.908 -0.826
-0.908 1.837 -0.552
-0.826 -0.552 3.090
28.245 5.380 2.845
5.380 30.237 3.396
2.845 3.396 23.597

orbtensor 34 H
-8.513 4.270 0.722
4.270 -13.818 0.122

0.722	0.122	-1.208
35.528	-1.286	-1.907
-1.286	34.985	-0.619
-1.907	-0.619	20.363

orbtensor 35 H

-18.305	0.194	2.079
0.194	-3.345	0.048
2.079	0.048	-2.224
42.253	-0.368	-2.633
-0.368	30.338	-0.418
-2.633	-0.418	21.860

orbtensor 36 H

-8.516	7.871	0.264
7.871	-13.242	-0.478
0.264	-0.478	-3.218
34.452	-6.970	-1.067
-6.970	38.072	0.111
-1.067	0.111	23.368

orbtensor 37 H

-4.881	-4.747	0.679
-4.747	-16.705	1.405
0.679	1.405	-1.688
31.365	1.205	-1.286
1.205	40.413	-1.132
-1.286	-1.132	22.025

orbtensor 38 Cr

-5040.523	401.164	-78.879
401.164	-3571.210	-152.519
-78.879	-152.519	-5474.863
1810.105	-0.348	0.235
-0.348	1811.894	0.041
0.235	0.041	1811.770

orbtensor 39 Br

-872.955	-63.954	-2.676
-63.954	-1078.710	449.779
-2.676	449.779	-931.661
3090.062	-1.761	-3.348
-1.761	3096.688	8.392
-3.348	8.392	3099.539

orbtensor 40 Br

-870.735	-171.804	11.366
-171.804	-1167.968	-394.655
11.366	-394.655	-844.601
3092.386	-3.294	5.700
-3.294	3095.028	-7.374
5.700	-7.374	3098.875

gtensor (ppt)

-0.154	0.005	0.000
0.005	-0.156	-0.001
0.000	-0.001	-0.155
14.173	8.034	-1.802
8.034	13.646	-1.568
-1.802	-1.568	3.701

zfstensor (cm-1)

-0.558512	0.552787	0.197239
0.552787	-0.167110	-0.119526
0.197239	-0.119526	0.725622

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.5657	-38.04667	4727.41276	-7.23885	4720.17392	4682.12725
2	C	3.5383	24.03267	-1873.80593	4.87597	-1868.92996	-1844.89729
3	C	-0.6670	58.00667	353.22522	-2.65268	350.57253	408.57920
4	C	1.2263	45.49767	-649.43307	5.81129	-643.62178	-598.12411
5	C	-1.1093	49.43967	587.47302	-1.25558	586.21744	635.65711
6	C	0.5177	23.34800	-274.14231	0.19137	-273.95094	-250.60294
7	C	0.2357	53.30867	-124.80271	1.03622	-123.76649	-70.45783
8	C	-0.3597	53.31900	190.46977	-0.75996	189.70981	243.02881
9	C	-0.7720	48.25700	408.83038	1.31146	410.14184	458.39884
10	C	0.6347	43.01800	-336.10235	-1.95027	-338.05262	-295.03462
11	C	-0.4747	54.82567	251.37067	0.85678	252.22745	307.05311
12	C	1.3117	60.46200	-694.62330	0.89274	-693.73056	-633.26856
13	C	1.1397	60.66533	-603.53674	-1.09614	-604.63288	-543.96754
14	C	1.3117	60.46633	-694.62330	0.01311	-694.61019	-634.14386
15	C	0.4753	169.91733	-251.72372	1.51826	-250.20546	-80.28813
16	H	0.8073	29.54367	-107.52844	0.33441	-107.19403	-77.65036
17	H	0.1737	29.79900	-23.13060	0.67348	-22.45712	7.34188
18	H	-0.0003	28.44067	0.04440	1.60174	1.64613	30.08680
19	C	0.3597	170.43067	-190.46977	-0.45209	-190.92185	-20.49119
20	H	-0.6677	29.59867	88.92629	-0.27158	88.65470	118.25337
21	H	-0.1943	28.53267	25.88319	0.16377	26.04696	54.57963
22	H	-0.1193	29.20300	15.89396	-0.83930	15.05467	44.25767
23	C	0.3603	170.42833	-190.82282	-0.45463	-191.27745	-20.84911
24	C	0.4747	169.91467	-251.37067	1.15640	-250.21427	-80.29961
25	H	0.8067	29.54300	-107.43965	0.19285	-107.24680	-77.70380
26	H	-0.0013	28.43900	0.17759	1.41521	1.59279	30.03179
27	H	0.1737	29.79800	-23.13060	0.40192	-22.72868	7.06932
28	H	0.6493	24.04133	-86.48448	-0.48010	-86.96457	-62.92324
29	H	-1.3933	23.35900	185.57757	-0.32980	185.24778	208.60678
30	C	1.1387	60.66667	-603.00716	-1.29034	-604.29750	-543.63083
31	H	-0.1193	29.20300	15.89396	-0.81808	15.07589	44.27889
32	H	-0.1937	28.53233	25.79439	0.19076	25.98515	54.51749
33	H	-0.6673	29.59833	88.88189	-0.29822	88.58367	118.18200
34	H	-1.6037	22.44567	213.59180	-1.34175	212.25005	234.69572
35	H	-0.4133	23.52567	55.05172	-0.20817	54.84355	78.36922
36	H	0.0890	23.63867	-11.85388	-0.15213	-12.00601	11.63265
37	H	-0.2647	23.50967	35.25086	-0.16037	35.09049	58.60016
38	Cr	21.4360	-2884.27567	50409.20408	14.59561	50423.79969	47539.52402
39	Br	5.4057	2134.32100	-2863.83066	-61.06994	-2924.90059	-790.57959
40	Br	5.4113	2134.32833	-2866.83276	-73.90744	-2940.74020	-806.41187

=====
CrL2-STO-PBE-No-ZFS
Temperature: 298
Spin: 1.5

atensor 1 N
-1.643 0.256 -0.223
0.256 -2.421 -0.078
-0.223 -0.078 -3.246
0.002 0.015 0.001
0.002 0.013 0.000
0.002 -0.002 0.019

atensor 2 C
2.725 0.977 0.379
0.977 1.996 0.090
0.379 0.090 6.037
-0.060 -0.014 0.009
0.076 0.065 -0.013
0.004 -0.001 0.006

atensor 3 C

0.248 0.178 -0.259
0.178 -0.378 -0.092
-0.259 -0.092 -1.664
0.005 -0.004 0.000
0.006 -0.003 -0.001
-0.001 0.001 0.000

atensor 4 C
0.185 0.096 0.496
0.096 -0.378 0.224
0.496 0.224 4.033
0.003 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.589 -0.078 -0.124
-0.078 -1.049 -0.018
-0.124 -0.018 -1.573
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.061
-0.446 -0.658 0.132
-0.061 0.132 0.777
0.014 -0.011 -0.002
-0.015 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.124 -0.100 0.081
-0.100 -0.146 0.058
0.081 0.058 0.706
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.123 -0.152 -0.063
-0.152 -0.218 -0.005
-0.063 -0.005 -0.669
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.057 -0.250 0.125
-0.250 -0.943 0.072
0.125 0.072 -0.203
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.287 -0.944 -0.163
-0.944 0.900 0.053
-0.163 0.053 -0.360
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.234 -1.496 0.022
-1.496 -1.773 0.274
0.022 0.274 -0.230

0.044 0.002 0.002
0.001 0.010 0.003
0.002 0.002 0.061

atensor 12 C
0.191 -0.462 0.081
-0.462 2.194 -2.301
0.081 -2.301 1.377
0.014 0.013 -0.013
-0.032 0.011 -0.026
-0.006 0.014 0.043

atensor 13 C
1.747 1.612 -0.795
1.612 0.355 -1.067
-0.795 -1.067 1.154
0.023 0.019 -0.008
-0.023 0.028 0.025
0.007 0.003 0.072

atensor 14 C
0.223 0.122 0.175
0.122 2.670 2.208
0.175 2.208 0.869
0.021 0.011 0.018
-0.023 0.012 0.036
0.015 -0.014 0.034

atensor 15 C
-0.022 -0.230 0.312
-0.230 0.388 -0.772
0.312 -0.772 1.053
0.004 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.063 -0.201 0.248
-0.201 1.367 -1.390
0.248 -1.390 1.264
-0.008 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.109 -1.201 1.610
-1.201 -0.182 -1.691
1.610 -1.691 0.785
-0.009 -0.008 0.004
-0.011 -0.004 -0.005
0.003 0.006 -0.002

atensor 18 H
-1.789 -0.240 0.520
-0.240 -1.063 -1.723
0.520 -1.723 2.907
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.009 -0.005

atensor 19 C
0.477 0.430 -0.603
0.430 0.078 -0.390
-0.603 -0.390 0.426
0.002 0.000 -0.002
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.613 0.933 -0.823
0.933 -0.450 -0.867
-0.823 -0.867 -0.699
0.006 0.006 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.310 0.834 -2.141
0.833 -1.381 -1.082
-2.141 -1.082 1.179
0.002 0.000 -0.023
0.007 0.002 -0.015
-0.002 0.007 -0.001

atensor 22 H
1.499 1.167 -1.473
1.167 -1.091 -0.592
-1.473 -0.592 -0.787
0.016 0.001 -0.012
0.009 0.002 -0.006
-0.005 0.001 0.000

atensor 23 C
0.753 0.573 0.454
0.573 0.150 0.275
0.454 0.275 0.079
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.105 -0.037 -0.018
-0.037 0.560 0.865
-0.018 0.865 0.963
0.005 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.104 0.144 0.073
0.144 1.657 1.360
0.073 1.360 1.013
-0.007 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.751 0.258 0.639
0.258 -0.659 2.103
0.639 2.104 2.465
-0.016 -0.009 0.010
-0.003 0.000 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.815 -0.868 -1.132
-0.868 0.212 2.058
-1.132 2.058 1.098
-0.010 -0.009 -0.001
-0.010 -0.004 0.007
0.000 -0.003 -0.001

atensor 28 H
1.359 0.658 -0.222

0.658 0.520 -0.117
-0.222 -0.117 -0.076
0.008 0.002 -0.001
0.009 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
0.016 0.346 -0.222
0.346 -2.361 -0.003
-0.222 -0.003 -1.552
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.047 1.897 0.349
1.897 0.539 0.663
0.349 0.663 0.670
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.036 1.388 0.589
1.388 -1.001 0.253
0.589 0.253 -1.416
0.019 0.002 0.006
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.796 1.331 2.095
1.331 -1.158 0.993
2.095 0.993 -0.147
0.008 0.001 0.020
0.010 0.002 0.012
-0.002 -0.008 -0.007

atensor 33 H
-0.248 1.189 0.571
1.189 -0.301 0.532
0.571 0.532 -1.213
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.390 2.872 -0.466
2.872 0.771 -0.610
-0.466 -0.610 -3.765
0.036 0.066 -0.006
0.013 -0.008 0.000
-0.003 -0.007 0.017

atensor 35 H
0.235 -0.259 -0.106
-0.259 -0.696 0.033
-0.106 0.033 -0.690
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.337 -0.372 -0.055
-0.372 0.106 0.029
-0.055 0.029 -0.240
0.000 -0.002 0.000

-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.474 -0.629 -0.003
-0.629 0.530 0.013
-0.003 0.013 -0.759
-0.006 -0.005 0.001
-0.007 -0.001 0.001
0.001 0.001 0.000

atensor 38 Cr
17.763 2.563 -0.262
2.563 27.076 -0.869
-0.262 -0.869 16.849
0.181 -0.809 0.320
-0.825 0.724 0.191
0.321 0.189 2.303

atensor 39 Br
31.364 1.560 10.672
1.560 12.066 -26.335
10.672 -26.335 -28.686
-1.119 -0.250 -0.494
-0.229 -0.073 2.492
-0.812 1.945 3.016

atensor 40 Br
22.194 5.699 -24.961
5.699 17.050 20.947
-24.961 20.947 -24.480
-0.520 -0.583 1.516
-0.666 -0.492 -2.031
1.837 -1.493 2.838

orbtensor 1 N
-479.281 54.193 47.135
54.193 -548.298 17.272
47.135 17.272 -95.205
338.950 -3.912 -2.104
-3.912 349.532 -1.007
-2.104 -1.007 321.202

orbtensor 2 C
-272.176 26.129 24.527
26.129 -297.150 8.628
24.527 8.628 -73.148
252.700 5.872 -5.674
5.872 251.509 -2.895
-5.674 -2.895 211.609

orbtensor 3 C
-218.840 -44.958 23.581
-44.958 -287.439 18.083
23.581 18.083 -56.822
251.907 3.527 -3.929
3.527 262.827 -2.566
-3.929 -2.566 223.256

orbtensor 4 C
-299.347 -23.670 32.717
-23.670 -231.580 12.411
32.717 12.411 -57.951
256.820 3.289 -5.332
3.289 252.550 -2.319
-5.332 -2.319 217.260

orbtensor 5 C
-287.705 2.937 29.715
2.937 -275.558 11.275
29.715 11.275 -58.400
269.107 0.351 -4.438
0.351 266.574 -1.730
-4.438 -1.730 235.192

orbtensor 6 C
-274.267 20.946 21.576
20.946 -295.338 7.761
21.576 7.761 -100.045
263.029 -5.222 -5.644
-5.222 260.585 -1.639
-5.644 -1.639 217.536

orbtensor 7 C
-295.948 10.219 30.106
10.219 -208.949 6.725
30.106 6.725 -60.365
257.825 -4.261 -5.049
-4.261 251.200 -1.276
-5.049 -1.276 217.278

orbtensor 8 C
-250.135 55.071 23.052
55.071 -267.464 4.543
23.052 4.543 -50.322
253.524 -5.982 -4.040
-5.982 255.586 -1.135
-4.040 -1.135 220.032

orbtensor 9 C
-233.115 -33.883 24.689
-33.883 -291.370 16.815
24.689 16.815 -57.952
252.258 -3.871 -4.140
-3.871 257.197 -1.551
-4.140 -1.551 218.891

orbtensor 10 C
-300.853 -15.896 28.364
-15.896 -249.616 10.658
28.364 10.658 -89.723
269.558 -1.101 -4.369
-1.101 264.629 -1.421
-4.369 -1.421 235.565

orbtensor 11 C
-215.744 32.161 -0.363
32.161 -130.730 -8.038
-0.363 -8.038 -204.884
244.708 -9.330 -0.978
-9.330 239.946 0.840
-0.978 0.840 233.305

orbtensor 12 C
-198.056 18.023 0.264
18.023 -104.706 24.875
0.264 24.875 -233.062
240.641 -2.865 -4.611
-2.865 236.236 -7.096
-4.611 -7.096 242.356

orbtensor 13 C
-225.505 -9.616 13.739
-9.616 -93.147 13.957

13.739	13.957	-217.880
244.227	5.169	-1.508
5.169	233.499	-4.824
-1.508	-4.824	243.006

orbtensor 14 C

-200.663	9.022	-9.333
9.022	-111.682	-41.081
-9.333	-41.081	-223.467
243.012	-0.449	4.416
-0.449	237.825	7.874
4.416	7.874	238.396

orbtensor 15 C

-55.887	0.656	6.495
0.656	-46.626	3.063
6.495	3.063	-49.104
218.375	-0.791	2.847
-0.791	218.006	-4.437
2.847	-4.437	227.668

orbtensor 16 H

3.272	-0.645	0.015
-0.645	2.115	1.320
0.015	1.320	1.644
23.114	0.381	-0.259
0.381	29.431	-6.854
-0.259	-6.854	28.921

orbtensor 17 H

3.527	0.497	-2.080
0.497	3.542	2.370
-2.080	2.370	3.000
29.854	-0.400	0.643
-0.400	20.927	-2.462
0.643	-2.462	28.407

orbtensor 18 H

5.131	0.391	-0.151
0.391	3.452	2.285
-0.151	2.285	-1.150
21.019	-3.201	-0.403
-3.201	26.847	0.717
-0.403	0.717	29.887

orbtensor 19 C

-53.363	-0.598	-5.764
-0.598	-44.732	2.486
-5.764	2.486	-54.379
225.407	1.728	-6.938
1.728	218.455	-1.653
-6.938	-1.653	222.584

orbtensor 20 H

2.417	-0.595	1.036
-0.595	2.165	0.783
1.036	0.783	2.585
26.266	3.906	-3.914
3.906	29.148	-5.084
-3.914	-5.084	26.091

orbtensor 21 H

2.745	-1.622	2.707
-1.622	3.694	1.143
2.707	1.143	0.376
25.121	3.575	-3.023
3.575	25.224	2.652

-3.023 2.652 28.308

orbtensor 22 H

-0.719 -1.236 1.411
-1.236 3.061 1.230
1.411 1.230 3.804
33.255 -1.325 -0.769
-1.325 22.582 -1.396
-0.769 -1.396 25.503

orbtensor 23 C

-50.594 -0.774 4.927
-0.774 -45.354 -3.415
4.927 -3.415 -56.534
228.542 2.765 5.103
2.765 218.779 1.300
5.103 1.300 219.127

orbtensor 24 C

-58.613 -0.703 -3.936
-0.703 -47.286 -3.088
-3.936 -3.088 -45.726
217.568 0.310 -0.323
0.310 219.050 5.469
-0.323 5.469 227.432

orbtensor 25 H

3.187 -0.978 -0.295
-0.978 1.855 -1.132
-0.295 -1.132 1.987
23.552 2.162 1.336
2.162 30.821 6.312
1.336 6.312 27.093

orbtensor 26 H

4.814 -0.316 -1.337
-0.316 2.922 -2.719
-1.337 -2.719 -0.305
21.856 -3.068 2.836
-3.068 26.817 0.383
2.836 0.383 29.077

orbtensor 27 H

4.506 0.077 1.722
0.077 3.029 -2.501
1.722 -2.501 2.531
29.443 0.241 -0.976
0.241 21.526 3.229
-0.976 3.229 28.219

orbtensor 28 H

-5.457 -5.975 0.655
-5.975 -16.999 1.511
0.655 1.511 -2.956
32.075 4.802 -1.359
4.802 41.552 -1.567
-1.359 -1.567 23.675

orbtensor 29 H

-18.330 -3.029 2.300
-3.029 -3.552 0.491
2.300 0.491 -1.901
41.554 2.357 -2.727
2.357 30.543 -0.793
-2.727 -0.793 21.581

orbtensor 30 C

-231.320	-15.583	-8.442
-15.583	-97.080	-23.139
-8.442	-23.139	-208.107
244.712	6.428	0.313
6.428	234.449	4.205
0.313	4.205	241.556

orbtensor 31 H

-1.078	-1.565	0.039
-1.565	2.851	-0.742
0.039	-0.742	4.372
33.162	-0.917	-1.144
-0.917	22.938	1.947
-1.144	1.947	25.241

orbtensor 32 H

1.331	-2.182	-2.720
-2.182	3.473	-0.908
-2.720	-0.908	2.010
26.717	3.158	3.151
3.158	24.605	-3.206
3.151	-3.206	27.333

orbtensor 33 H

1.945	-0.860	-0.771
-0.860	2.027	-0.509
-0.771	-0.509	3.197
28.024	5.361	2.786
5.361	30.047	3.373
2.786	3.373	23.433

orbtensor 34 H

-8.516	4.227	0.728
4.227	-13.872	0.132
0.728	0.132	-1.182
35.495	-1.233	-1.913
-1.233	34.956	-0.627
-1.913	-0.627	20.304

orbtensor 35 H

-18.350	0.182	2.085
0.182	-3.315	0.048
2.085	0.048	-2.224
42.132	-0.344	-2.627
-0.344	30.316	-0.423
-2.627	-0.423	21.796

orbtensor 36 H

-8.514	7.941	0.250
7.941	-13.307	-0.488
0.250	-0.488	-3.295
34.389	-6.946	-1.061
-6.946	38.028	0.110
-1.061	0.110	23.364

orbtensor 37 H

-4.778	-4.832	0.662
-4.832	-16.721	1.414
0.662	1.414	-1.745
31.233	1.248	-1.274
1.248	40.303	-1.133
-1.274	-1.133	22.000

orbtensor 38 Cr

-5086.458	406.347	-81.052
406.347	-3608.278	-154.448
-81.052	-154.448	-5535.483

1810.272 -0.430 0.294
 -0.430 1811.483 0.105
 0.294 0.105 1812.357

orbtensor 39 Br
 -862.313 -61.921 -1.700
 -61.921 -1070.541 443.108
 -1.700 443.108 -926.543
 3090.320 -1.622 -3.292
 -1.622 3096.312 7.776
 -3.292 7.776 3099.372

orbtensor 40 Br
 -861.021 -168.382 8.723
 -168.382 -1158.553 -389.141
 8.723 -389.141 -839.913
 3092.580 -3.016 5.510
 -3.016 3094.777 -6.800
 5.510 -6.800 3098.645

gtensor (ppt)
 -0.154 0.005 0.000
 0.005 -0.155 0.000
 0.000 0.000 -0.153
 13.944 8.045 -1.814
 8.045 13.446 -1.575
 -1.814 -1.575 3.383

averaging
 2H Average:34
 4H Average:29
 9,10H Average:16,17,18,20,21,22
 5H Average:35
 8,11H Average:25,26,27,31,32,33
 6H Average:36
 3H Average:28
 7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.4253	-37.70000	4468.29301	-4.20142	4464.09159	4426.39159
2	C	3.5897	24.44800	-1900.75834	0.92755	-1899.83078	-1875.38278
3	C	-0.5973	58.29633	316.29296	-1.33921	314.95375	373.25009
4	C	1.2737	45.91733	-674.41709	2.56945	-671.84763	-625.93030
5	C	-1.0677	49.73667	565.33837	-0.39916	564.93921	614.67588
6	C	0.5123	23.83333	-271.28476	0.85541	-270.42934	-246.59601
7	C	0.2263	53.68033	-119.84538	0.61155	-119.23383	-65.55350
8	C	-0.3357	53.74033	177.73829	-0.11249	177.62580	231.36613
9	C	-0.7387	48.63633	391.13014	0.91374	392.04387	440.68021
10	C	0.6070	43.18667	-321.41155	0.42680	-320.98475	-277.79808
11	C	-0.5513	55.53367	291.93558	2.49546	294.43104	349.96470
12	C	1.2767	61.13633	-676.00561	0.22456	-675.78105	-614.64472
13	C	1.1263	61.40000	-596.40286	-2.75771	-599.16057	-537.76057
14	C	1.2763	61.14033	-675.82911	0.22594	-675.60317	-614.46284
15	C	0.4763	170.81067	-252.22246	0.74679	-251.47567	-80.66500
16	H	0.8550	29.49900	-113.86323	0.09605	-113.76718	-84.26818
17	H	0.1597	29.75233	-21.26335	0.58296	-20.68039	9.07194
18	H	0.0107	28.39533	-1.42052	0.67119	-0.74932	27.64601
19	C	0.3313	171.32400	-175.44375	-0.82320	-176.26695	-4.94295
20	H	-0.5837	29.55733	77.72886	-0.48523	77.24363	106.80096
21	H	-0.1697	28.48933	22.59508	-0.24444	22.35064	50.83997
22	H	-0.1203	29.16200	16.02520	-0.74205	15.28314	44.44514
23	C	0.3317	171.32200	-175.62026	-0.82426	-176.44451	-5.12251
24	C	0.4760	170.80833	-252.04596	0.74584	-251.30012	-80.49178

25	H	0.8543	29.49833	-113.77445	0.09570	-113.67875	-84.18041
26	H	0.0110	28.39367	-1.46491	0.67114	-0.79377	27.59990
27	H	0.1600	29.75133	-21.30774	0.58293	-20.72480	9.02653
28	H	0.6060	23.96333	-80.70306	-0.42094	-81.12400	-57.16067
29	H	-1.2980	23.29833	172.85903	-0.21140	172.64763	195.94597
30	C	1.1263	61.40333	-596.40286	-2.75851	-599.16137	-537.75803
31	H	-0.1210	29.16200	16.11398	-0.74228	15.37170	44.53370
32	H	-0.1687	28.48967	22.46191	-0.24458	22.21733	50.70699
33	H	-0.5837	29.55767	77.72886	-0.48546	77.24339	106.80106
34	H	-1.4463	22.39500	192.61308	-1.62611	190.98697	213.38197
35	H	-0.3830	23.45167	51.00540	0.01158	51.01698	74.46864
36	H	0.0673	23.55500	-8.96701	0.05926	-8.90775	14.64725
37	H	-0.2367	23.43067	31.51770	0.11308	31.63078	55.06145
38	Cr	21.6320	-2932.03567	50863.90310	20.69955	50884.60265	47952.56698
39	Br	5.5227	2142.20233	-2925.45768	-33.95977	-2959.41745	-817.21512
40	Br	5.5300	2142.17167	-2929.34228	-33.97138	-2963.31366	-821.14199

=====
 CrL2-STO-PBE-Neese
 Temperature: 298
 Spin: 1.5

atensor 1 N
 -1.643 0.256 -0.223
 0.256 -2.421 -0.078
 -0.223 -0.078 -3.246
 0.002 0.015 0.001
 0.002 0.013 0.000
 0.002 -0.002 0.019

atensor 2 C
 2.725 0.977 0.379
 0.977 1.996 0.090
 0.379 0.090 6.037
 -0.060 -0.014 0.009
 0.076 0.065 -0.013
 0.004 -0.001 0.006

atensor 3 C
 0.248 0.178 -0.259
 0.178 -0.378 -0.092
 -0.259 -0.092 -1.664
 0.005 -0.004 0.000
 0.006 -0.003 -0.001
 -0.001 0.001 0.000

atensor 4 C
 0.185 0.096 0.496
 0.096 -0.378 0.224
 0.496 0.224 4.033
 0.003 0.010 -0.001
 -0.015 -0.021 0.003
 0.000 0.000 -0.001

atensor 5 C
 -0.589 -0.078 -0.124
 -0.078 -1.049 -0.018
 -0.124 -0.018 -1.573
 0.003 -0.003 0.000
 0.000 0.005 0.000
 0.000 0.000 0.000

atensor 6 C
 1.436 -0.446 -0.061
 -0.446 -0.658 0.132
 -0.061 0.132 0.777

0.014 -0.011 -0.002
-0.015 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.124 -0.100 0.081
-0.100 -0.146 0.058
0.081 0.058 0.706
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.123 -0.152 -0.063
-0.152 -0.218 -0.005
-0.063 -0.005 -0.669
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.057 -0.250 0.125
-0.250 -0.943 0.072
0.125 0.072 -0.203
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.287 -0.944 -0.163
-0.944 0.900 0.053
-0.163 0.053 -0.360
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.234 -1.496 0.022
-1.496 -1.773 0.274
0.022 0.274 -0.230
0.044 0.002 0.002
0.001 0.010 0.003
0.002 0.002 0.061

atensor 12 C
0.191 -0.462 0.081
-0.462 2.194 -2.301
0.081 -2.301 1.377
0.014 0.013 -0.013
-0.032 0.011 -0.026
-0.006 0.014 0.043

atensor 13 C
1.747 1.612 -0.795
1.612 0.355 -1.067
-0.795 -1.067 1.154
0.023 0.019 -0.008
-0.023 0.028 0.025
0.007 0.003 0.072

atensor 14 C
0.223 0.122 0.175
0.122 2.670 2.208
0.175 2.208 0.869
0.021 0.011 0.018
-0.023 0.012 0.036
0.015 -0.014 0.034

atensor 15 C
-0.022 -0.230 0.312
-0.230 0.388 -0.772
0.312 -0.772 1.053
0.004 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.063 -0.201 0.248
-0.201 1.367 -1.390
0.248 -1.390 1.264
-0.008 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.109 -1.201 1.610
-1.201 -0.182 -1.691
1.610 -1.691 0.785
-0.009 -0.008 0.004
-0.011 -0.004 -0.005
0.003 0.006 -0.002

atensor 18 H
-1.789 -0.240 0.520
-0.240 -1.063 -1.723
0.520 -1.723 2.907
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.009 -0.005

atensor 19 C
0.477 0.430 -0.603
0.430 0.078 -0.390
-0.603 -0.390 0.426
0.002 0.000 -0.002
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.613 0.933 -0.823
0.933 -0.450 -0.867
-0.823 -0.867 -0.699
0.006 0.006 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.310 0.834 -2.141
0.833 -1.381 -1.082
-2.141 -1.082 1.179
0.002 0.000 -0.023
0.007 0.002 -0.015
-0.002 0.007 -0.001

atensor 22 H
1.499 1.167 -1.473
1.167 -1.091 -0.592
-1.473 -0.592 -0.787
0.016 0.001 -0.012
0.009 0.002 -0.006
-0.005 0.001 0.000

atensor 23 C
0.753 0.573 0.454

0.573 0.150 0.275
0.454 0.275 0.079
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.105 -0.037 -0.018
-0.037 0.560 0.865
-0.018 0.865 0.963
0.005 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.104 0.144 0.073
0.144 1.657 1.360
0.073 1.360 1.013
-0.007 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.751 0.258 0.639
0.258 -0.659 2.103
0.639 2.104 2.465
-0.016 -0.009 0.010
-0.003 0.000 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.815 -0.868 -1.132
-0.868 0.212 2.058
-1.132 2.058 1.098
-0.010 -0.009 -0.001
-0.010 -0.004 0.007
0.000 -0.003 -0.001

atensor 28 H
1.359 0.658 -0.222
0.658 0.520 -0.117
-0.222 -0.117 -0.076
0.008 0.002 -0.001
0.009 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
0.016 0.346 -0.222
0.346 -2.361 -0.003
-0.222 -0.003 -1.552
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.047 1.897 0.349
1.897 0.539 0.663
0.349 0.663 0.670
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.036 1.388 0.589
1.388 -1.001 0.253
0.589 0.253 -1.416
0.019 0.002 0.006

0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.796 1.331 2.095
1.331 -1.158 0.993
2.095 0.993 -0.147
0.008 0.001 0.020
0.010 0.002 0.012
-0.002 -0.008 -0.007

atensor 33 H
-0.248 1.189 0.571
1.189 -0.301 0.532
0.571 0.532 -1.213
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.390 2.872 -0.466
2.872 0.771 -0.610
-0.466 -0.610 -3.765
0.036 0.066 -0.006
0.013 -0.008 0.000
-0.003 -0.007 0.017

atensor 35 H
0.235 -0.259 -0.106
-0.259 -0.696 0.033
-0.106 0.033 -0.690
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.337 -0.372 -0.055
-0.372 0.106 0.029
-0.055 0.029 -0.240
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.474 -0.629 -0.003
-0.629 0.530 0.013
-0.003 0.013 -0.759
-0.006 -0.005 0.001
-0.007 -0.001 0.001
0.001 0.001 0.000

atensor 38 Cr
17.763 2.563 -0.262
2.563 27.076 -0.869
-0.262 -0.869 16.849
0.181 -0.809 0.320
-0.825 0.724 0.191
0.321 0.189 2.303

atensor 39 Br
31.364 1.560 10.672
1.560 12.066 -26.335
10.672 -26.335 -28.686
-1.119 -0.250 -0.494
-0.229 -0.073 2.492
-0.812 1.945 3.016

atensor 40 Br
22.194 5.699 -24.961
5.699 17.050 20.947
-24.961 20.947 -24.480
-0.520 -0.583 1.516
-0.666 -0.492 -2.031
1.837 -1.493 2.838

orbtensor 1 N
-479.281 54.193 47.135
54.193 -548.298 17.272
47.135 17.272 -95.205
338.950 -3.912 -2.104
-3.912 349.532 -1.007
-2.104 -1.007 321.202

orbtensor 2 C
-272.176 26.129 24.527
26.129 -297.150 8.628
24.527 8.628 -73.148
252.700 5.872 -5.674
5.872 251.509 -2.895
-5.674 -2.895 211.609

orbtensor 3 C
-218.840 -44.958 23.581
-44.958 -287.439 18.083
23.581 18.083 -56.822
251.907 3.527 -3.929
3.527 262.827 -2.566
-3.929 -2.566 223.256

orbtensor 4 C
-299.347 -23.670 32.717
-23.670 -231.580 12.411
32.717 12.411 -57.951
256.820 3.289 -5.332
3.289 252.550 -2.319
-5.332 -2.319 217.260

orbtensor 5 C
-287.705 2.937 29.715
2.937 -275.558 11.275
29.715 11.275 -58.400
269.107 0.351 -4.438
0.351 266.574 -1.730
-4.438 -1.730 235.192

orbtensor 6 C
-274.267 20.946 21.576
20.946 -295.338 7.761
21.576 7.761 -100.045
263.029 -5.222 -5.644
-5.222 260.585 -1.639
-5.644 -1.639 217.536

orbtensor 7 C
-295.948 10.219 30.106
10.219 -208.949 6.725
30.106 6.725 -60.365
257.825 -4.261 -5.049
-4.261 251.200 -1.276
-5.049 -1.276 217.278

orbtensor 8 C
-250.135 55.071 23.052
55.071 -267.464 4.543

23.052	4.543	-50.322
253.524	-5.982	-4.040
-5.982	255.586	-1.135
-4.040	-1.135	220.032

orbtensor 9 C

-233.115	-33.883	24.689
-33.883	-291.370	16.815
24.689	16.815	-57.952
252.258	-3.871	-4.140
-3.871	257.197	-1.551
-4.140	-1.551	218.891

orbtensor 10 C

-300.853	-15.896	28.364
-15.896	-249.616	10.658
28.364	10.658	-89.723
269.558	-1.101	-4.369
-1.101	264.629	-1.421
-4.369	-1.421	235.565

orbtensor 11 C

-215.744	32.161	-0.363
32.161	-130.730	-8.038
-0.363	-8.038	-204.884
244.708	-9.330	-0.978
-9.330	239.946	0.840
-0.978	0.840	233.305

orbtensor 12 C

-198.056	18.023	0.264
18.023	-104.706	24.875
0.264	24.875	-233.062
240.641	-2.865	-4.611
-2.865	236.236	-7.096
-4.611	-7.096	242.356

orbtensor 13 C

-225.505	-9.616	13.739
-9.616	-93.147	13.957
13.739	13.957	-217.880
244.227	5.169	-1.508
5.169	233.499	-4.824
-1.508	-4.824	243.006

orbtensor 14 C

-200.663	9.022	-9.333
9.022	-111.682	-41.081
-9.333	-41.081	-223.467
243.012	-0.449	4.416
-0.449	237.825	7.874
4.416	7.874	238.396

orbtensor 15 C

-55.887	0.656	6.495
0.656	-46.626	3.063
6.495	3.063	-49.104
218.375	-0.791	2.847
-0.791	218.006	-4.437
2.847	-4.437	227.668

orbtensor 16 H

3.272	-0.645	0.015
-0.645	2.115	1.320
0.015	1.320	1.644
23.114	0.381	-0.259
0.381	29.431	-6.854

-0.259 -6.854 28.921

orbtensor 17 H

3.527 0.497 -2.080
0.497 3.542 2.370
-2.080 2.370 3.000
29.854 -0.400 0.643
-0.400 20.927 -2.462
0.643 -2.462 28.407

orbtensor 18 H

5.131 0.391 -0.151
0.391 3.452 2.285
-0.151 2.285 -1.150
21.019 -3.201 -0.403
-3.201 26.847 0.717
-0.403 0.717 29.887

orbtensor 19 C

-53.363 -0.598 -5.764
-0.598 -44.732 2.486
-5.764 2.486 -54.379
225.407 1.728 -6.938
1.728 218.455 -1.653
-6.938 -1.653 222.584

orbtensor 20 H

2.417 -0.595 1.036
-0.595 2.165 0.783
1.036 0.783 2.585
26.266 3.906 -3.914
3.906 29.148 -5.084
-3.914 -5.084 26.091

orbtensor 21 H

2.745 -1.622 2.707
-1.622 3.694 1.143
2.707 1.143 0.376
25.121 3.575 -3.023
3.575 25.224 2.652
-3.023 2.652 28.308

orbtensor 22 H

-0.719 -1.236 1.411
-1.236 3.061 1.230
1.411 1.230 3.804
33.255 -1.325 -0.769
-1.325 22.582 -1.396
-0.769 -1.396 25.503

orbtensor 23 C

-50.594 -0.774 4.927
-0.774 -45.354 -3.415
4.927 -3.415 -56.534
228.542 2.765 5.103
2.765 218.779 1.300
5.103 1.300 219.127

orbtensor 24 C

-58.613 -0.703 -3.936
-0.703 -47.286 -3.088
-3.936 -3.088 -45.726
217.568 0.310 -0.323
0.310 219.050 5.469
-0.323 5.469 227.432

orbtensor 25 H

3.187	-0.978	-0.295
-0.978	1.855	-1.132
-0.295	-1.132	1.987
23.552	2.162	1.336
2.162	30.821	6.312
1.336	6.312	27.093

orbtensor 26 H

4.814	-0.316	-1.337
-0.316	2.922	-2.719
-1.337	-2.719	-0.305
21.856	-3.068	2.836
-3.068	26.817	0.383
2.836	0.383	29.077

orbtensor 27 H

4.506	0.077	1.722
0.077	3.029	-2.501
1.722	-2.501	2.531
29.443	0.241	-0.976
0.241	21.526	3.229
-0.976	3.229	28.219

orbtensor 28 H

-5.457	-5.975	0.655
-5.975	-16.999	1.511
0.655	1.511	-2.956
32.075	4.802	-1.359
4.802	41.552	-1.567
-1.359	-1.567	23.675

orbtensor 29 H

-18.330	-3.029	2.300
-3.029	-3.552	0.491
2.300	0.491	-1.901
41.554	2.357	-2.727
2.357	30.543	-0.793
-2.727	-0.793	21.581

orbtensor 30 C

-231.320	-15.583	-8.442
-15.583	-97.080	-23.139
-8.442	-23.139	-208.107
244.712	6.428	0.313
6.428	234.449	4.205
0.313	4.205	241.556

orbtensor 31 H

-1.078	-1.565	0.039
-1.565	2.851	-0.742
0.039	-0.742	4.372
33.162	-0.917	-1.144
-0.917	22.938	1.947
-1.144	1.947	25.241

orbtensor 32 H

1.331	-2.182	-2.720
-2.182	3.473	-0.908
-2.720	-0.908	2.010
26.717	3.158	3.151
3.158	24.605	-3.206
3.151	-3.206	27.333

orbtensor 33 H

1.945	-0.860	-0.771
-0.860	2.027	-0.509
-0.771	-0.509	3.197

28.024	5.361	2.786
5.361	30.047	3.373
2.786	3.373	23.433

orbtensor 34 H

-8.516	4.227	0.728
4.227	-13.872	0.132
0.728	0.132	-1.182
35.495	-1.233	-1.913
-1.233	34.956	-0.627
-1.913	-0.627	20.304

orbtensor 35 H

-18.350	0.182	2.085
0.182	-3.315	0.048
2.085	0.048	-2.224
42.132	-0.344	-2.627
-0.344	30.316	-0.423
-2.627	-0.423	21.796

orbtensor 36 H

-8.514	7.941	0.250
7.941	-13.307	-0.488
0.250	-0.488	-3.295
34.389	-6.946	-1.061
-6.946	38.028	0.110
-1.061	0.110	23.364

orbtensor 37 H

-4.778	-4.832	0.662
-4.832	-16.721	1.414
0.662	1.414	-1.745
31.233	1.248	-1.274
1.248	40.303	-1.133
-1.274	-1.133	22.000

orbtensor 38 Cr

-5086.458	406.347	-81.052
406.347	-3608.278	-154.448
-81.052	-154.448	-5535.483
1810.272	-0.430	0.294
-0.430	1811.483	0.105
0.294	0.105	1812.357

orbtensor 39 Br

-862.313	-61.921	-1.700
-61.921	-1070.541	443.108
-1.700	443.108	-926.543
3090.320	-1.622	-3.292
-1.622	3096.312	7.776
-3.292	7.776	3099.372

orbtensor 40 Br

-861.021	-168.382	8.723
-168.382	-1158.553	-389.141
8.723	-389.141	-839.913
3092.580	-3.016	5.510
-3.016	3094.777	-6.800
5.510	-6.800	3098.645

gtensor (ppt)

-0.154	0.005	0.000
0.005	-0.155	0.000
0.000	0.000	-0.153
13.944	8.045	-1.814
8.045	13.446	-1.575
-1.814	-1.575	3.383

```

zfstensor (cm-1)
-2.129992    0.766494    0.682084
 0.766494   -0.659124   -0.285520
 0.682084   -0.285520    2.789116

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.4253	-37.70000	4468.37172	-17.59255	4450.77917	4413.07917
2	C	3.5897	24.44800	-1900.79182	12.99901	-1887.79280	-1863.34480
3	C	-0.5973	58.29633	316.29854	-6.39706	309.90147	368.19781
4	C	1.2737	45.91733	-674.42897	14.60041	-659.82856	-613.91123
5	C	-1.0677	49.73667	565.34833	-3.18658	562.16175	611.89842
6	C	0.5123	23.83333	-271.28954	-0.51990	-271.80944	-247.97610
7	C	0.2263	53.68033	-119.84749	2.37145	-117.47604	-63.79571
8	C	-0.3357	53.74033	177.74142	-1.92314	175.81828	229.55862
9	C	-0.7387	48.63633	391.13703	3.01053	394.14756	442.78390
10	C	0.6070	43.18667	-321.41721	-5.73812	-327.15533	-283.96866
11	C	-0.5513	55.53367	291.94072	0.13156	292.07228	347.60595
12	C	1.2767	61.13633	-676.01752	3.05352	-672.96400	-611.82767
13	C	1.1263	61.40000	-596.41337	-1.36180	-597.77517	-536.37517
14	C	1.2763	61.14033	-675.84101	-0.37549	-676.21650	-615.07617
15	C	0.4763	170.81067	-252.22690	4.04687	-248.18003	-77.36937
16	H	0.8550	29.49900	-113.86524	1.02105	-112.84419	-83.34519
17	H	0.1597	29.75233	-21.26372	1.57699	-19.68673	10.06560
18	H	0.0107	28.39533	-1.42054	4.25320	2.83266	31.22800
19	C	0.3313	171.32400	-175.44684	-0.63331	-176.08015	-4.75615
20	H	-0.5837	29.55733	77.73022	-0.37201	77.35821	106.91555
21	H	-0.1697	28.48933	22.59548	0.73250	23.32798	51.81732
22	H	-0.1203	29.16200	16.02548	-1.92307	14.10241	43.26441
23	C	0.3317	171.32200	-175.62335	-0.96254	-176.58589	-5.26389
24	C	0.4760	170.80833	-252.05040	2.74888	-249.30152	-78.49318
25	H	0.8543	29.49833	-113.77645	0.48486	-113.29159	-83.79326
26	H	0.0110	28.39367	-1.46493	3.52254	2.05761	30.45127
27	H	0.1600	29.75133	-21.30811	0.74212	-20.56600	9.18534
28	H	0.6060	23.96333	-80.70448	-1.11108	-81.81556	-57.85223
29	H	-1.2980	23.29833	172.86208	-0.87771	171.98437	195.28270
30	C	1.1263	61.40333	-596.41337	-2.46722	-598.88059	-537.47725
31	H	-0.1210	29.16200	16.11426	-1.99797	14.11629	43.27829
32	H	-0.1687	28.48967	22.46230	0.51370	22.97601	51.46567
33	H	-0.5837	29.55767	77.73022	-0.58210	77.14812	106.70579
34	H	-1.4463	22.39500	192.61647	-2.62833	189.98815	212.38315
35	H	-0.3830	23.45167	51.00630	-0.63829	50.36801	73.81967
36	H	0.0673	23.55500	-8.96716	-0.48462	-9.45179	14.10321
37	H	-0.2367	23.43067	31.51825	-0.50780	31.01046	54.44112
38	Cr	21.6320	-2932.03567	50864.79908	20.49653	50885.29560	47953.25994
39	Br	5.5227	2142.20233	-2925.50921	-150.80815	-3076.31737	-934.11503
40	Br	5.5300	2142.17167	-2929.39388	-189.50183	-3118.89571	-976.72405

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CrL2-STO-PBE-ORCA  

Temperature: 298  

Spin: 1.5

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atensor 1 N  

-1.643 0.256 -0.223  

0.256 -2.421 -0.078  

-0.223 -0.078 -3.246  

0.002 0.015 0.001  

0.002 0.013 0.000  

0.002 -0.002 0.019

```

```

atensor 2 C  

2.725 0.977 0.379

```

0.977 1.996 0.090
0.379 0.090 6.037
-0.060 -0.014 0.009
0.076 0.065 -0.013
0.004 -0.001 0.006

atensor 3 C
0.248 0.178 -0.259
0.178 -0.378 -0.092
-0.259 -0.092 -1.664
0.005 -0.004 0.000
0.006 -0.003 -0.001
-0.001 0.001 0.000

atensor 4 C
0.185 0.096 0.496
0.096 -0.378 0.224
0.496 0.224 4.033
0.003 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.589 -0.078 -0.124
-0.078 -1.049 -0.018
-0.124 -0.018 -1.573
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.061
-0.446 -0.658 0.132
-0.061 0.132 0.777
0.014 -0.011 -0.002
-0.015 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.124 -0.100 0.081
-0.100 -0.146 0.058
0.081 0.058 0.706
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.123 -0.152 -0.063
-0.152 -0.218 -0.005
-0.063 -0.005 -0.669
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.057 -0.250 0.125
-0.250 -0.943 0.072
0.125 0.072 -0.203
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.287 -0.944 -0.163
-0.944 0.900 0.053
-0.163 0.053 -0.360
0.002 -0.014 0.001

-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.234 -1.496 0.022
-1.496 -1.773 0.274
0.022 0.274 -0.230
0.044 0.002 0.002
0.001 0.010 0.003
0.002 0.002 0.061

atensor 12 C
0.191 -0.462 0.081
-0.462 2.194 -2.301
0.081 -2.301 1.377
0.014 0.013 -0.013
-0.032 0.011 -0.026
-0.006 0.014 0.043

atensor 13 C
1.747 1.612 -0.795
1.612 0.355 -1.067
-0.795 -1.067 1.154
0.023 0.019 -0.008
-0.023 0.028 0.025
0.007 0.003 0.072

atensor 14 C
0.223 0.122 0.175
0.122 2.670 2.208
0.175 2.208 0.869
0.021 0.011 0.018
-0.023 0.012 0.036
0.015 -0.014 0.034

atensor 15 C
-0.022 -0.230 0.312
-0.230 0.388 -0.772
0.312 -0.772 1.053
0.004 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.063 -0.201 0.248
-0.201 1.367 -1.390
0.248 -1.390 1.264
-0.008 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.109 -1.201 1.610
-1.201 -0.182 -1.691
1.610 -1.691 0.785
-0.009 -0.008 0.004
-0.011 -0.004 -0.005
0.003 0.006 -0.002

atensor 18 H
-1.789 -0.240 0.520
-0.240 -1.063 -1.723
0.520 -1.723 2.907
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.009 -0.005

atensor 19 C
0.477 0.430 -0.603
0.430 0.078 -0.390
-0.603 -0.390 0.426
0.002 0.000 -0.002
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.613 0.933 -0.823
0.933 -0.450 -0.867
-0.823 -0.867 -0.699
0.006 0.006 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.310 0.834 -2.141
0.833 -1.381 -1.082
-2.141 -1.082 1.179
0.002 0.000 -0.023
0.007 0.002 -0.015
-0.002 0.007 -0.001

atensor 22 H
1.499 1.167 -1.473
1.167 -1.091 -0.592
-1.473 -0.592 -0.787
0.016 0.001 -0.012
0.009 0.002 -0.006
-0.005 0.001 0.000

atensor 23 C
0.753 0.573 0.454
0.573 0.150 0.275
0.454 0.275 0.079
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.105 -0.037 -0.018
-0.037 0.560 0.865
-0.018 0.865 0.963
0.005 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.104 0.144 0.073
0.144 1.657 1.360
0.073 1.360 1.013
-0.007 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.751 0.258 0.639
0.258 -0.659 2.103
0.639 2.104 2.465
-0.016 -0.009 0.010
-0.003 0.000 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.815 -0.868 -1.132
-0.868 0.212 2.058

-1.132 2.058 1.098
-0.010 -0.009 -0.001
-0.010 -0.004 0.007
0.000 -0.003 -0.001

atensor 28 H
1.359 0.658 -0.222
0.658 0.520 -0.117
-0.222 -0.117 -0.076
0.008 0.002 -0.001
0.009 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
0.016 0.346 -0.222
0.346 -2.361 -0.003
-0.222 -0.003 -1.552
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.047 1.897 0.349
1.897 0.539 0.663
0.349 0.663 0.670
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.036 1.388 0.589
1.388 -1.001 0.253
0.589 0.253 -1.416
0.019 0.002 0.006
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.796 1.331 2.095
1.331 -1.158 0.993
2.095 0.993 -0.147
0.008 0.001 0.020
0.010 0.002 0.012
-0.002 -0.008 -0.007

atensor 33 H
-0.248 1.189 0.571
1.189 -0.301 0.532
0.571 0.532 -1.213
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.390 2.872 -0.466
2.872 0.771 -0.610
-0.466 -0.610 -3.765
0.036 0.066 -0.006
0.013 -0.008 0.000
-0.003 -0.007 0.017

atensor 35 H
0.235 -0.259 -0.106
-0.259 -0.696 0.033
-0.106 0.033 -0.690
0.003 -0.002 0.000
-0.001 -0.002 0.000

0.000 0.000 0.001

atensor 36 H
0.337 -0.372 -0.055
-0.372 0.106 0.029
-0.055 0.029 -0.240
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.474 -0.629 -0.003
-0.629 0.530 0.013
-0.003 0.013 -0.759
-0.006 -0.005 0.001
-0.007 -0.001 0.001
0.001 0.001 0.000

atensor 38 Cr
17.763 2.563 -0.262
2.563 27.076 -0.869
-0.262 -0.869 16.849
0.181 -0.809 0.320
-0.825 0.724 0.191
0.321 0.189 2.303

atensor 39 Br
31.364 1.560 10.672
1.560 12.066 -26.335
10.672 -26.335 -28.686
-1.119 -0.250 -0.494
-0.229 -0.073 2.492
-0.812 1.945 3.016

atensor 40 Br
22.194 5.699 -24.961
5.699 17.050 20.947
-24.961 20.947 -24.480
-0.520 -0.583 1.516
-0.666 -0.492 -2.031
1.837 -1.493 2.838

orbtensor 1 N
-479.281 54.193 47.135
54.193 -548.298 17.272
47.135 17.272 -95.205
338.950 -3.912 -2.104
-3.912 349.532 -1.007
-2.104 -1.007 321.202

orbtensor 2 C
-272.176 26.129 24.527
26.129 -297.150 8.628
24.527 8.628 -73.148
252.700 5.872 -5.674
5.872 251.509 -2.895
-5.674 -2.895 211.609

orbtensor 3 C
-218.840 -44.958 23.581
-44.958 -287.439 18.083
23.581 18.083 -56.822
251.907 3.527 -3.929
3.527 262.827 -2.566
-3.929 -2.566 223.256

orbtensor 4 C

-299.347	-23.670	32.717
-23.670	-231.580	12.411
32.717	12.411	-57.951
256.820	3.289	-5.332
3.289	252.550	-2.319
-5.332	-2.319	217.260

orbtensor 5 C

-287.705	2.937	29.715
2.937	-275.558	11.275
29.715	11.275	-58.400
269.107	0.351	-4.438
0.351	266.574	-1.730
-4.438	-1.730	235.192

orbtensor 6 C

-274.267	20.946	21.576
20.946	-295.338	7.761
21.576	7.761	-100.045
263.029	-5.222	-5.644
-5.222	260.585	-1.639
-5.644	-1.639	217.536

orbtensor 7 C

-295.948	10.219	30.106
10.219	-208.949	6.725
30.106	6.725	-60.365
257.825	-4.261	-5.049
-4.261	251.200	-1.276
-5.049	-1.276	217.278

orbtensor 8 C

-250.135	55.071	23.052
55.071	-267.464	4.543
23.052	4.543	-50.322
253.524	-5.982	-4.040
-5.982	255.586	-1.135
-4.040	-1.135	220.032

orbtensor 9 C

-233.115	-33.883	24.689
-33.883	-291.370	16.815
24.689	16.815	-57.952
252.258	-3.871	-4.140
-3.871	257.197	-1.551
-4.140	-1.551	218.891

orbtensor 10 C

-300.853	-15.896	28.364
-15.896	-249.616	10.658
28.364	10.658	-89.723
269.558	-1.101	-4.369
-1.101	264.629	-1.421
-4.369	-1.421	235.565

orbtensor 11 C

-215.744	32.161	-0.363
32.161	-130.730	-8.038
-0.363	-8.038	-204.884
244.708	-9.330	-0.978
-9.330	239.946	0.840
-0.978	0.840	233.305

orbtensor 12 C

-198.056	18.023	0.264
18.023	-104.706	24.875
0.264	24.875	-233.062

240.641	-2.865	-4.611
-2.865	236.236	-7.096
-4.611	-7.096	242.356

orbtensor 13 C

-225.505	-9.616	13.739
-9.616	-93.147	13.957
13.739	13.957	-217.880
244.227	5.169	-1.508
5.169	233.499	-4.824
-1.508	-4.824	243.006

orbtensor 14 C

-200.663	9.022	-9.333
9.022	-111.682	-41.081
-9.333	-41.081	-223.467
243.012	-0.449	4.416
-0.449	237.825	7.874
4.416	7.874	238.396

orbtensor 15 C

-55.887	0.656	6.495
0.656	-46.626	3.063
6.495	3.063	-49.104
218.375	-0.791	2.847
-0.791	218.006	-4.437
2.847	-4.437	227.668

orbtensor 16 H

3.272	-0.645	0.015
-0.645	2.115	1.320
0.015	1.320	1.644
23.114	0.381	-0.259
0.381	29.431	-6.854
-0.259	-6.854	28.921

orbtensor 17 H

3.527	0.497	-2.080
0.497	3.542	2.370
-2.080	2.370	3.000
29.854	-0.400	0.643
-0.400	20.927	-2.462
0.643	-2.462	28.407

orbtensor 18 H

5.131	0.391	-0.151
0.391	3.452	2.285
-0.151	2.285	-1.150
21.019	-3.201	-0.403
-3.201	26.847	0.717
-0.403	0.717	29.887

orbtensor 19 C

-53.363	-0.598	-5.764
-0.598	-44.732	2.486
-5.764	2.486	-54.379
225.407	1.728	-6.938
1.728	218.455	-1.653
-6.938	-1.653	222.584

orbtensor 20 H

2.417	-0.595	1.036
-0.595	2.165	0.783
1.036	0.783	2.585
26.266	3.906	-3.914
3.906	29.148	-5.084
-3.914	-5.084	26.091

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orbtensor 21 H
2.745   -1.622   2.707
-1.622   3.694   1.143
2.707   1.143   0.376
25.121   3.575  -3.023
3.575   25.224  2.652
-3.023   2.652  28.308

orbtensor 22 H
-0.719  -1.236   1.411
-1.236   3.061   1.230
1.411   1.230   3.804
33.255  -1.325  -0.769
-1.325  22.582  -1.396
-0.769  -1.396  25.503

orbtensor 23 C
-50.594  -0.774   4.927
-0.774  -45.354  -3.415
4.927  -3.415  -56.534
228.542   2.765   5.103
2.765  218.779   1.300
5.103   1.300  219.127

orbtensor 24 C
-58.613  -0.703  -3.936
-0.703  -47.286  -3.088
-3.936  -3.088  -45.726
217.568   0.310  -0.323
0.310  219.050   5.469
-0.323   5.469  227.432

orbtensor 25 H
3.187  -0.978  -0.295
-0.978   1.855  -1.132
-0.295  -1.132   1.987
23.552   2.162   1.336
2.162  30.821   6.312
1.336   6.312  27.093

orbtensor 26 H
4.814  -0.316  -1.337
-0.316   2.922  -2.719
-1.337  -2.719  -0.305
21.856  -3.068   2.836
-3.068  26.817   0.383
2.836   0.383  29.077

orbtensor 27 H
4.506   0.077   1.722
0.077   3.029  -2.501
1.722  -2.501   2.531
29.443   0.241  -0.976
0.241  21.526   3.229
-0.976   3.229  28.219

orbtensor 28 H
-5.457  -5.975   0.655
-5.975  -16.999   1.511
0.655   1.511  -2.956
32.075   4.802  -1.359
4.802  41.552  -1.567
-1.359  -1.567  23.675

orbtensor 29 H
-18.330  -3.029   2.300

```

-3.029	-3.552	0.491
2.300	0.491	-1.901
41.554	2.357	-2.727
2.357	30.543	-0.793
-2.727	-0.793	21.581

orbtensor 30 C

-231.320	-15.583	-8.442
-15.583	-97.080	-23.139
-8.442	-23.139	-208.107
244.712	6.428	0.313
6.428	234.449	4.205
0.313	4.205	241.556

orbtensor 31 H

-1.078	-1.565	0.039
-1.565	2.851	-0.742
0.039	-0.742	4.372
33.162	-0.917	-1.144
-0.917	22.938	1.947
-1.144	1.947	25.241

orbtensor 32 H

1.331	-2.182	-2.720
-2.182	3.473	-0.908
-2.720	-0.908	2.010
26.717	3.158	3.151
3.158	24.605	-3.206
3.151	-3.206	27.333

orbtensor 33 H

1.945	-0.860	-0.771
-0.860	2.027	-0.509
-0.771	-0.509	3.197
28.024	5.361	2.786
5.361	30.047	3.373
2.786	3.373	23.433

orbtensor 34 H

-8.516	4.227	0.728
4.227	-13.872	0.132
0.728	0.132	-1.182
35.495	-1.233	-1.913
-1.233	34.956	-0.627
-1.913	-0.627	20.304

orbtensor 35 H

-18.350	0.182	2.085
0.182	-3.315	0.048
2.085	0.048	-2.224
42.132	-0.344	-2.627
-0.344	30.316	-0.423
-2.627	-0.423	21.796

orbtensor 36 H

-8.514	7.941	0.250
7.941	-13.307	-0.488
0.250	-0.488	-3.295
34.389	-6.946	-1.061
-6.946	38.028	0.110
-1.061	0.110	23.364

orbtensor 37 H

-4.778	-4.832	0.662
-4.832	-16.721	1.414
0.662	1.414	-1.745
31.233	1.248	-1.274

1.248 40.303 -1.133
 -1.274 -1.133 22.000

orbtensor 38 Cr
 -5086.458 406.347 -81.052
 406.347 -3608.278 -154.448
 -81.052 -154.448 -5535.483
 1810.272 -0.430 0.294
 -0.430 1811.483 0.105
 0.294 0.105 1812.357

orbtensor 39 Br
 -862.313 -61.921 -1.700
 -61.921 -1070.541 443.108
 -1.700 443.108 -926.543
 3090.320 -1.622 -3.292
 -1.622 3096.312 7.776
 -3.292 7.776 3099.372

orbtensor 40 Br
 -861.021 -168.382 8.723
 -168.382 -1158.553 -389.141
 8.723 -389.141 -839.913
 3092.580 -3.016 5.510
 -3.016 3094.777 -6.800
 5.510 -6.800 3098.645

gtensor (ppt)
 -0.154 0.005 0.000
 0.005 -0.155 0.000
 0.000 0.000 -0.153
 13.944 8.045 -1.814
 8.045 13.446 -1.575
 -1.814 -1.575 3.383

zfstensor (cm-1)
 -9.155671 -0.807368 0.702096
 -0.807368 -7.468741 0.280503
 0.702096 0.280503 -4.103457

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.4253	-37.70000	4468.48928	-21.29582	4447.19346	4409.49346
2	C	3.5897	24.44800	-1900.84183	9.87332	-1890.96850	-1866.52050
3	C	-0.5973	58.29633	316.30686	-7.19621	309.11065	367.40698
4	C	1.2737	45.91733	-674.44671	14.60491	-659.84180	-613.92446
5	C	-1.0677	49.73667	565.36321	-3.02323	562.33997	612.07664
6	C	0.5123	23.83333	-271.29667	0.88598	-270.41070	-246.57736
7	C	0.2263	53.68033	-119.85065	2.75150	-117.09914	-63.41881
8	C	-0.3357	53.74033	177.74610	-1.46779	176.27831	230.01864
9	C	-0.7387	48.63633	391.14732	3.96941	395.11673	443.75307
10	C	0.6070	43.18667	-321.42566	-2.68403	-324.10969	-280.92303
11	C	-0.5513	55.53367	291.94841	5.05844	297.00684	352.54051
12	C	1.2767	61.13633	-676.03530	2.13130	-673.90401	-612.76767
13	C	1.1263	61.40000	-596.42906	-7.95771	-604.38676	-542.98676
14	C	1.2763	61.14033	-675.85879	2.08558	-673.77322	-612.63288
15	C	0.4763	170.81067	-252.23354	3.98138	-248.25216	-77.44149
16	H	0.8550	29.49900	-113.86823	0.82543	-113.04280	-83.54380
17	H	0.1597	29.75233	-21.26428	2.08756	-19.17673	10.57561
18	H	0.0107	28.39533	-1.42058	4.00060	2.58002	30.97535
19	C	0.3313	171.32400	-175.45146	-2.53670	-177.98816	-6.66416
20	H	-0.5837	29.55733	77.73227	-1.39236	76.33991	105.89725
21	H	-0.1697	28.48933	22.59607	-0.30561	22.29047	50.77980
22	H	-0.1203	29.16200	16.02590	-3.14087	12.88503	42.04703
23	C	0.3317	171.32200	-175.62797	-2.54628	-178.17425	-6.85225

24	C	0.4760	170.80833	-252.05703	3.96177	-248.09526	-77.28693
25	H	0.8543	29.49833	-113.77944	0.81686	-112.96258	-83.46425
26	H	0.0110	28.39367	-1.46497	3.98940	2.52443	30.91810
27	H	0.1600	29.75133	-21.30867	2.07708	-19.23160	10.51974
28	H	0.6060	23.96333	-80.70661	-1.71468	-82.42129	-58.45795
29	H	-1.2980	23.29833	172.86662	-1.22943	171.63720	194.93553
30	C	1.1263	61.40333	-596.42906	-7.97589	-604.40495	-543.00162
31	H	-0.1210	29.16200	16.11469	-3.14344	12.97125	42.13325
32	H	-0.1687	28.48967	22.46289	-0.31113	22.15176	50.64143
33	H	-0.5837	29.55767	77.73227	-1.39690	76.33537	105.89304
34	H	-1.4463	22.39500	192.62154	-5.13294	187.48860	209.88360
35	H	-0.3830	23.45167	51.00764	-0.44706	50.56058	74.01225
36	H	0.0673	23.55500	-8.96740	-0.18239	-9.14979	14.40521
37	H	-0.2367	23.43067	31.51908	0.03506	31.55414	54.98481
38	Cr	21.6320	-2932.03567	50866.13730	44.49296	50910.63026	47978.59460
39	Br	5.5227	2142.20233	-2925.58618	-185.56185	-3111.14803	-968.94569
40	Br	5.5300	2142.17167	-2929.47095	-186.11626	-3115.58721	-973.41555

=====
 CrL2-STO-PBE-Pederson
 Temperature: 298
 Spin: 1.5

atensor 1 N
 -1.643 0.256 -0.223
 0.256 -2.421 -0.078
 -0.223 -0.078 -3.246
 0.002 0.015 0.001
 0.002 0.013 0.000
 0.002 -0.002 0.019

atensor 2 C
 2.725 0.977 0.379
 0.977 1.996 0.090
 0.379 0.090 6.037
 -0.060 -0.014 0.009
 0.076 0.065 -0.013
 0.004 -0.001 0.006

atensor 3 C
 0.248 0.178 -0.259
 0.178 -0.378 -0.092
 -0.259 -0.092 -1.664
 0.005 -0.004 0.000
 0.006 -0.003 -0.001
 -0.001 0.001 0.000

atensor 4 C
 0.185 0.096 0.496
 0.096 -0.378 0.224
 0.496 0.224 4.033
 0.003 0.010 -0.001
 -0.015 -0.021 0.003
 0.000 0.000 -0.001

atensor 5 C
 -0.589 -0.078 -0.124
 -0.078 -1.049 -0.018
 -0.124 -0.018 -1.573
 0.003 -0.003 0.000
 0.000 0.005 0.000
 0.000 0.000 0.000

atensor 6 C
 1.436 -0.446 -0.061
 -0.446 -0.658 0.132

-0.061 0.132 0.777
0.014 -0.011 -0.002
-0.015 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.124 -0.100 0.081
-0.100 -0.146 0.058
0.081 0.058 0.706
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.123 -0.152 -0.063
-0.152 -0.218 -0.005
-0.063 -0.005 -0.669
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.057 -0.250 0.125
-0.250 -0.943 0.072
0.125 0.072 -0.203
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.287 -0.944 -0.163
-0.944 0.900 0.053
-0.163 0.053 -0.360
0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.234 -1.496 0.022
-1.496 -1.773 0.274
0.022 0.274 -0.230
0.044 0.002 0.002
0.001 0.010 0.003
0.002 0.002 0.061

atensor 12 C
0.191 -0.462 0.081
-0.462 2.194 -2.301
0.081 -2.301 1.377
0.014 0.013 -0.013
-0.032 0.011 -0.026
-0.006 0.014 0.043

atensor 13 C
1.747 1.612 -0.795
1.612 0.355 -1.067
-0.795 -1.067 1.154
0.023 0.019 -0.008
-0.023 0.028 0.025
0.007 0.003 0.072

atensor 14 C
0.223 0.122 0.175
0.122 2.670 2.208
0.175 2.208 0.869
0.021 0.011 0.018
-0.023 0.012 0.036

0.015 -0.014 0.034

atensor 15 C
-0.022 -0.230 0.312
-0.230 0.388 -0.772
0.312 -0.772 1.053
0.004 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.063 -0.201 0.248
-0.201 1.367 -1.390
0.248 -1.390 1.264
-0.008 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.109 -1.201 1.610
-1.201 -0.182 -1.691
1.610 -1.691 0.785
-0.009 -0.008 0.004
-0.011 -0.004 -0.005
0.003 0.006 -0.002

atensor 18 H
-1.789 -0.240 0.520
-0.240 -1.063 -1.723
0.520 -1.723 2.907
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.009 -0.005

atensor 19 C
0.477 0.430 -0.603
0.430 0.078 -0.390
-0.603 -0.390 0.426
0.002 0.000 -0.002
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.613 0.933 -0.823
0.933 -0.450 -0.867
-0.823 -0.867 -0.699
0.006 0.006 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.310 0.834 -2.141
0.833 -1.381 -1.082
-2.141 -1.082 1.179
0.002 0.000 -0.023
0.007 0.002 -0.015
-0.002 0.007 -0.001

atensor 22 H
1.499 1.167 -1.473
1.167 -1.091 -0.592
-1.473 -0.592 -0.787
0.016 0.001 -0.012
0.009 0.002 -0.006
-0.005 0.001 0.000

atensor 23 C

0.753 0.573 0.454
0.573 0.150 0.275
0.454 0.275 0.079
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.105 -0.037 -0.018
-0.037 0.560 0.865
-0.018 0.865 0.963
0.005 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.104 0.144 0.073
0.144 1.657 1.360
0.073 1.360 1.013
-0.007 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.751 0.258 0.639
0.258 -0.659 2.103
0.639 2.104 2.465
-0.016 -0.009 0.010
-0.003 0.000 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.815 -0.868 -1.132
-0.868 0.212 2.058
-1.132 2.058 1.098
-0.010 -0.009 -0.001
-0.010 -0.004 0.007
0.000 -0.003 -0.001

atensor 28 H
1.359 0.658 -0.222
0.658 0.520 -0.117
-0.222 -0.117 -0.076
0.008 0.002 -0.001
0.009 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
0.016 0.346 -0.222
0.346 -2.361 -0.003
-0.222 -0.003 -1.552
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.047 1.897 0.349
1.897 0.539 0.663
0.349 0.663 0.670
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.036 1.388 0.589
1.388 -1.001 0.253
0.589 0.253 -1.416

0.019 0.002 0.006
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.796 1.331 2.095
1.331 -1.158 0.993
2.095 0.993 -0.147
0.008 0.001 0.020
0.010 0.002 0.012
-0.002 -0.008 -0.007

atensor 33 H
-0.248 1.189 0.571
1.189 -0.301 0.532
0.571 0.532 -1.213
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.390 2.872 -0.466
2.872 0.771 -0.610
-0.466 -0.610 -3.765
0.036 0.066 -0.006
0.013 -0.008 0.000
-0.003 -0.007 0.017

atensor 35 H
0.235 -0.259 -0.106
-0.259 -0.696 0.033
-0.106 0.033 -0.690
0.003 -0.002 0.000
-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.337 -0.372 -0.055
-0.372 0.106 0.029
-0.055 0.029 -0.240
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.474 -0.629 -0.003
-0.629 0.530 0.013
-0.003 0.013 -0.759
-0.006 -0.005 0.001
-0.007 -0.001 0.001
0.001 0.001 0.000

atensor 38 Cr
17.763 2.563 -0.262
2.563 27.076 -0.869
-0.262 -0.869 16.849
0.181 -0.809 0.320
-0.825 0.724 0.191
0.321 0.189 2.303

atensor 39 Br
31.364 1.560 10.672
1.560 12.066 -26.335
10.672 -26.335 -28.686
-1.119 -0.250 -0.494
-0.229 -0.073 2.492
-0.812 1.945 3.016

atensor 40 Br
22.194 5.699 -24.961
5.699 17.050 20.947
-24.961 20.947 -24.480
-0.520 -0.583 1.516
-0.666 -0.492 -2.031
1.837 -1.493 2.838

orbtensor 1 N
-479.281 54.193 47.135
54.193 -548.298 17.272
47.135 17.272 -95.205
338.950 -3.912 -2.104
-3.912 349.532 -1.007
-2.104 -1.007 321.202

orbtensor 2 C
-272.176 26.129 24.527
26.129 -297.150 8.628
24.527 8.628 -73.148
252.700 5.872 -5.674
5.872 251.509 -2.895
-5.674 -2.895 211.609

orbtensor 3 C
-218.840 -44.958 23.581
-44.958 -287.439 18.083
23.581 18.083 -56.822
251.907 3.527 -3.929
3.527 262.827 -2.566
-3.929 -2.566 223.256

orbtensor 4 C
-299.347 -23.670 32.717
-23.670 -231.580 12.411
32.717 12.411 -57.951
256.820 3.289 -5.332
3.289 252.550 -2.319
-5.332 -2.319 217.260

orbtensor 5 C
-287.705 2.937 29.715
2.937 -275.558 11.275
29.715 11.275 -58.400
269.107 0.351 -4.438
0.351 266.574 -1.730
-4.438 -1.730 235.192

orbtensor 6 C
-274.267 20.946 21.576
20.946 -295.338 7.761
21.576 7.761 -100.045
263.029 -5.222 -5.644
-5.222 260.585 -1.639
-5.644 -1.639 217.536

orbtensor 7 C
-295.948 10.219 30.106
10.219 -208.949 6.725
30.106 6.725 -60.365
257.825 -4.261 -5.049
-4.261 251.200 -1.276
-5.049 -1.276 217.278

orbtensor 8 C
-250.135 55.071 23.052

55.071	-267.464	4.543
23.052	4.543	-50.322
253.524	-5.982	-4.040
-5.982	255.586	-1.135
-4.040	-1.135	220.032

orbtensor 9 C

-233.115	-33.883	24.689
-33.883	-291.370	16.815
24.689	16.815	-57.952
252.258	-3.871	-4.140
-3.871	257.197	-1.551
-4.140	-1.551	218.891

orbtensor 10 C

-300.853	-15.896	28.364
-15.896	-249.616	10.658
28.364	10.658	-89.723
269.558	-1.101	-4.369
-1.101	264.629	-1.421
-4.369	-1.421	235.565

orbtensor 11 C

-215.744	32.161	-0.363
32.161	-130.730	-8.038
-0.363	-8.038	-204.884
244.708	-9.330	-0.978
-9.330	239.946	0.840
-0.978	0.840	233.305

orbtensor 12 C

-198.056	18.023	0.264
18.023	-104.706	24.875
0.264	24.875	-233.062
240.641	-2.865	-4.611
-2.865	236.236	-7.096
-4.611	-7.096	242.356

orbtensor 13 C

-225.505	-9.616	13.739
-9.616	-93.147	13.957
13.739	13.957	-217.880
244.227	5.169	-1.508
5.169	233.499	-4.824
-1.508	-4.824	243.006

orbtensor 14 C

-200.663	9.022	-9.333
9.022	-111.682	-41.081
-9.333	-41.081	-223.467
243.012	-0.449	4.416
-0.449	237.825	7.874
4.416	7.874	238.396

orbtensor 15 C

-55.887	0.656	6.495
0.656	-46.626	3.063
6.495	3.063	-49.104
218.375	-0.791	2.847
-0.791	218.006	-4.437
2.847	-4.437	227.668

orbtensor 16 H

3.272	-0.645	0.015
-0.645	2.115	1.320
0.015	1.320	1.644
23.114	0.381	-0.259

0.381	29.431	-6.854
-0.259	-6.854	28.921

orbtensor 17 H

3.527	0.497	-2.080
0.497	3.542	2.370
-2.080	2.370	3.000
29.854	-0.400	0.643
-0.400	20.927	-2.462
0.643	-2.462	28.407

orbtensor 18 H

5.131	0.391	-0.151
0.391	3.452	2.285
-0.151	2.285	-1.150
21.019	-3.201	-0.403
-3.201	26.847	0.717
-0.403	0.717	29.887

orbtensor 19 C

-53.363	-0.598	-5.764
-0.598	-44.732	2.486
-5.764	2.486	-54.379
225.407	1.728	-6.938
1.728	218.455	-1.653
-6.938	-1.653	222.584

orbtensor 20 H

2.417	-0.595	1.036
-0.595	2.165	0.783
1.036	0.783	2.585
26.266	3.906	-3.914
3.906	29.148	-5.084
-3.914	-5.084	26.091

orbtensor 21 H

2.745	-1.622	2.707
-1.622	3.694	1.143
2.707	1.143	0.376
25.121	3.575	-3.023
3.575	25.224	2.652
-3.023	2.652	28.308

orbtensor 22 H

-0.719	-1.236	1.411
-1.236	3.061	1.230
1.411	1.230	3.804
33.255	-1.325	-0.769
-1.325	22.582	-1.396
-0.769	-1.396	25.503

orbtensor 23 C

-50.594	-0.774	4.927
-0.774	-45.354	-3.415
4.927	-3.415	-56.534
228.542	2.765	5.103
2.765	218.779	1.300
5.103	1.300	219.127

orbtensor 24 C

-58.613	-0.703	-3.936
-0.703	-47.286	-3.088
-3.936	-3.088	-45.726
217.568	0.310	-0.323
0.310	219.050	5.469
-0.323	5.469	227.432

orbtensor 25 H
3.187 -0.978 -0.295
-0.978 1.855 -1.132
-0.295 -1.132 1.987
23.552 2.162 1.336
2.162 30.821 6.312
1.336 6.312 27.093

orbtensor 26 H
4.814 -0.316 -1.337
-0.316 2.922 -2.719
-1.337 -2.719 -0.305
21.856 -3.068 2.836
-3.068 26.817 0.383
2.836 0.383 29.077

orbtensor 27 H
4.506 0.077 1.722
0.077 3.029 -2.501
1.722 -2.501 2.531
29.443 0.241 -0.976
0.241 21.526 3.229
-0.976 3.229 28.219

orbtensor 28 H
-5.457 -5.975 0.655
-5.975 -16.999 1.511
0.655 1.511 -2.956
32.075 4.802 -1.359
4.802 41.552 -1.567
-1.359 -1.567 23.675

orbtensor 29 H
-18.330 -3.029 2.300
-3.029 -3.552 0.491
2.300 0.491 -1.901
41.554 2.357 -2.727
2.357 30.543 -0.793
-2.727 -0.793 21.581

orbtensor 30 C
-231.320 -15.583 -8.442
-15.583 -97.080 -23.139
-8.442 -23.139 -208.107
244.712 6.428 0.313
6.428 234.449 4.205
0.313 4.205 241.556

orbtensor 31 H
-1.078 -1.565 0.039
-1.565 2.851 -0.742
0.039 -0.742 4.372
33.162 -0.917 -1.144
-0.917 22.938 1.947
-1.144 1.947 25.241

orbtensor 32 H
1.331 -2.182 -2.720
-2.182 3.473 -0.908
-2.720 -0.908 2.010
26.717 3.158 3.151
3.158 24.605 -3.206
3.151 -3.206 27.333

orbtensor 33 H
1.945 -0.860 -0.771
-0.860 2.027 -0.509

-0.771	-0.509	3.197
28.024	5.361	2.786
5.361	30.047	3.373
2.786	3.373	23.433

orbtensor 34 H

-8.516	4.227	0.728
4.227	-13.872	0.132
0.728	0.132	-1.182
35.495	-1.233	-1.913
-1.233	34.956	-0.627
-1.913	-0.627	20.304

orbtensor 35 H

-18.350	0.182	2.085
0.182	-3.315	0.048
2.085	0.048	-2.224
42.132	-0.344	-2.627
-0.344	30.316	-0.423
-2.627	-0.423	21.796

orbtensor 36 H

-8.514	7.941	0.250
7.941	-13.307	-0.488
0.250	-0.488	-3.295
34.389	-6.946	-1.061
-6.946	38.028	0.110
-1.061	0.110	23.364

orbtensor 37 H

-4.778	-4.832	0.662
-4.832	-16.721	1.414
0.662	1.414	-1.745
31.233	1.248	-1.274
1.248	40.303	-1.133
-1.274	-1.133	22.000

orbtensor 38 Cr

-5086.458	406.347	-81.052
406.347	-3608.278	-154.448
-81.052	-154.448	-5535.483
1810.272	-0.430	0.294
-0.430	1811.483	0.105
0.294	0.105	1812.357

orbtensor 39 Br

-862.313	-61.921	-1.700
-61.921	-1070.541	443.108
-1.700	443.108	-926.543
3090.320	-1.622	-3.292
-1.622	3096.312	7.776
-3.292	7.776	3099.372

orbtensor 40 Br

-861.021	-168.382	8.723
-168.382	-1158.553	-389.141
8.723	-389.141	-839.913
3092.580	-3.016	5.510
-3.016	3094.777	-6.800
5.510	-6.800	3098.645

gtensor (ppt)

-0.154	0.005	0.000
0.005	-0.155	0.000
0.000	0.000	-0.153
13.944	8.045	-1.814
8.045	13.446	-1.575

-1.814 -1.575 3.383

zfstensor (cm-1)

-0.377205 0.362896 0.131075
0.362896 -0.100603 -0.078015
0.131075 -0.078015 0.477809

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.4253	-37.70000	4468.29036	-6.09608	4462.19428	4424.49428
2	C	3.5897	24.44800	-1900.75721	3.47034	-1897.28687	-1872.83887
3	C	-0.5973	58.29633	316.29278	-2.12988	314.16289	372.45923
4	C	1.2737	45.91733	-674.41669	4.66601	-669.75068	-623.83334
5	C	-1.0677	49.73667	565.33804	-0.92229	564.41575	614.15242
6	C	0.5123	23.83333	-271.28460	0.36490	-270.91970	-247.08636
7	C	0.2263	53.68033	-119.84531	0.86030	-118.98501	-65.30467
8	C	-0.3357	53.74033	177.73818	-0.49647	177.24171	230.98205
9	C	-0.7387	48.63633	391.12991	1.14986	392.27977	440.91610
10	C	0.6070	43.18667	-321.41135	-1.09372	-322.50507	-279.31840
11	C	-0.5513	55.53367	291.93541	1.33940	293.27481	348.80848
12	C	1.2767	61.13633	-676.00521	0.65031	-675.35490	-614.21856
13	C	1.1263	61.40000	-596.40251	-1.73236	-598.13486	-536.73486
14	C	1.2763	61.14033	-675.82871	0.08227	-675.74644	-614.60611
15	C	0.4763	170.81067	-252.22231	1.26158	-250.96073	-80.15006
16	H	0.8550	29.49900	-113.86316	0.25755	-113.60561	-84.10661
17	H	0.1597	29.75233	-21.26334	0.64549	-20.61784	9.13449
18	H	0.0107	28.39533	-1.42052	1.28678	-0.13373	28.26160
19	C	0.3313	171.32400	-175.44365	-0.58616	-176.02981	-4.70581
20	H	-0.5837	29.55733	77.72881	-0.34627	77.38254	106.93988
21	H	-0.1697	28.48933	22.59507	0.01980	22.61487	51.10421
22	H	-0.1203	29.16200	16.02519	-0.81448	15.21071	44.37271
23	C	0.3317	171.32200	-175.62015	-0.58668	-176.20684	-4.88484
24	C	0.4760	170.80833	-252.04581	1.02650	-251.01930	-80.21097
25	H	0.8543	29.49833	-113.77438	0.16520	-113.60918	-84.11085
26	H	0.0110	28.39367	-1.46491	1.16575	-0.29916	28.09451
27	H	0.1600	29.75133	-21.30773	0.46947	-20.83826	8.91307
28	H	0.6060	23.96333	-80.70301	-0.46238	-81.16539	-57.20206
29	H	-1.2980	23.29833	172.85893	-0.29344	172.56549	195.86383
30	C	1.1263	61.40333	-596.40251	-1.85772	-598.26023	-536.85690
31	H	-0.1210	29.16200	16.11397	-0.79995	15.31402	44.47602
32	H	-0.1687	28.48967	22.46189	0.03890	22.50080	50.99047
33	H	-0.5837	29.55767	77.72881	-0.36317	77.36564	106.92331
34	H	-1.4463	22.39500	192.61297	-1.43733	191.17563	213.57063
35	H	-0.3830	23.45167	51.00537	-0.13502	50.87035	74.32202
36	H	0.0673	23.55500	-8.96700	-0.08005	-9.04706	14.50794
37	H	-0.2367	23.43067	31.51768	-0.06597	31.45171	54.88238
38	Cr	21.6320	-2932.03567	50863.87297	16.23568	50880.10865	47948.07298
39	Br	5.5227	2142.20233	-2925.45595	-51.82797	-2977.28392	-835.08158
40	Br	5.5300	2142.17167	-2929.34054	-60.06535	-2989.40590	-847.23423

=====
CrL2-STO-PBE-Van-Wullen

Temperature: 298

Spin: 1.5

atensor 1 N

-1.643 0.256 -0.223
0.256 -2.421 -0.078
-0.223 -0.078 -3.246
0.002 0.015 0.001
0.002 0.013 0.000
0.002 -0.002 0.019

atensor 2 C

2.725 0.977 0.379
0.977 1.996 0.090
0.379 0.090 6.037
-0.060 -0.014 0.009
0.076 0.065 -0.013
0.004 -0.001 0.006

atensor 3 C
0.248 0.178 -0.259
0.178 -0.378 -0.092
-0.259 -0.092 -1.664
0.005 -0.004 0.000
0.006 -0.003 -0.001
-0.001 0.001 0.000

atensor 4 C
0.185 0.096 0.496
0.096 -0.378 0.224
0.496 0.224 4.033
0.003 0.010 -0.001
-0.015 -0.021 0.003
0.000 0.000 -0.001

atensor 5 C
-0.589 -0.078 -0.124
-0.078 -1.049 -0.018
-0.124 -0.018 -1.573
0.003 -0.003 0.000
0.000 0.005 0.000
0.000 0.000 0.000

atensor 6 C
1.436 -0.446 -0.061
-0.446 -0.658 0.132
-0.061 0.132 0.777
0.014 -0.011 -0.002
-0.015 -0.029 0.003
-0.001 0.003 -0.003

atensor 7 C
0.124 -0.100 0.081
-0.100 -0.146 0.058
0.081 0.058 0.706
0.001 0.001 0.000
-0.002 -0.006 0.001
0.000 0.000 0.000

atensor 8 C
-0.123 -0.152 -0.063
-0.152 -0.218 -0.005
-0.063 -0.005 -0.669
0.000 0.003 0.000
0.000 0.003 0.000
0.000 -0.001 0.000

atensor 9 C
-1.057 -0.250 0.125
-0.250 -0.943 0.072
0.125 0.072 -0.203
-0.007 -0.014 0.002
-0.006 -0.005 0.001
0.001 0.002 -0.001

atensor 10 C
1.287 -0.944 -0.163
-0.944 0.900 0.053
-0.163 0.053 -0.360

0.002 -0.014 0.001
-0.004 -0.009 0.001
0.000 0.002 0.001

atensor 11 C
0.234 -1.496 0.022
-1.496 -1.773 0.274
0.022 0.274 -0.230
0.044 0.002 0.002
0.001 0.010 0.003
0.002 0.002 0.061

atensor 12 C
0.191 -0.462 0.081
-0.462 2.194 -2.301
0.081 -2.301 1.377
0.014 0.013 -0.013
-0.032 0.011 -0.026
-0.006 0.014 0.043

atensor 13 C
1.747 1.612 -0.795
1.612 0.355 -1.067
-0.795 -1.067 1.154
0.023 0.019 -0.008
-0.023 0.028 0.025
0.007 0.003 0.072

atensor 14 C
0.223 0.122 0.175
0.122 2.670 2.208
0.175 2.208 0.869
0.021 0.011 0.018
-0.023 0.012 0.036
0.015 -0.014 0.034

atensor 15 C
-0.022 -0.230 0.312
-0.230 0.388 -0.772
0.312 -0.772 1.053
0.004 0.000 -0.005
-0.004 0.003 -0.002
0.001 0.007 0.003

atensor 16 H
-0.063 -0.201 0.248
-0.201 1.367 -1.390
0.248 -1.390 1.264
-0.008 0.001 -0.006
-0.004 0.004 -0.010
0.005 0.002 0.001

atensor 17 H
-0.109 -1.201 1.610
-1.201 -0.182 -1.691
1.610 -1.691 0.785
-0.009 -0.008 0.004
-0.011 -0.004 -0.005
0.003 0.006 -0.002

atensor 18 H
-1.789 -0.240 0.520
-0.240 -1.063 -1.723
0.520 -1.723 2.907
-0.017 -0.008 -0.006
-0.006 -0.001 -0.014
0.008 0.009 -0.005

atensor 19 C
0.477 0.430 -0.603
0.430 0.078 -0.390
-0.603 -0.390 0.426
0.002 0.000 -0.002
-0.001 0.004 -0.003
-0.001 0.004 0.007

atensor 20 H
-0.613 0.933 -0.823
0.933 -0.450 -0.867
-0.823 -0.867 -0.699
0.006 0.006 -0.012
0.005 0.003 -0.007
-0.005 0.000 0.002

atensor 21 H
-0.310 0.834 -2.141
0.833 -1.381 -1.082
-2.141 -1.082 1.179
0.002 0.000 -0.023
0.007 0.002 -0.015
-0.002 0.007 -0.001

atensor 22 H
1.499 1.167 -1.473
1.167 -1.091 -0.592
-1.473 -0.592 -0.787
0.016 0.001 -0.012
0.009 0.002 -0.006
-0.005 0.001 0.000

atensor 23 C
0.753 0.573 0.454
0.573 0.150 0.275
0.454 0.275 0.079
0.003 0.000 0.003
0.000 0.004 0.003
0.002 -0.004 0.006

atensor 24 C
-0.105 -0.037 -0.018
-0.037 0.560 0.865
-0.018 0.865 0.963
0.005 -0.001 0.004
-0.003 0.002 0.003
-0.001 -0.007 0.003

atensor 25 H
-0.104 0.144 0.073
0.144 1.657 1.360
0.073 1.360 1.013
-0.007 0.001 0.008
-0.002 0.004 0.010
-0.002 -0.003 0.000

atensor 26 H
-1.751 0.258 0.639
0.258 -0.659 2.103
0.639 2.104 2.465
-0.016 -0.009 0.010
-0.003 0.000 0.015
-0.005 -0.007 -0.006

atensor 27 H
-0.815 -0.868 -1.132

-0.868 0.212 2.058
-1.132 2.058 1.098
-0.010 -0.009 -0.001
-0.010 -0.004 0.007
0.000 -0.003 -0.001

atensor 28 H
1.359 0.658 -0.222
0.658 0.520 -0.117
-0.222 -0.117 -0.076
0.008 0.002 -0.001
0.009 0.005 -0.001
-0.001 0.000 0.002

atensor 29 H
0.016 0.346 -0.222
0.346 -2.361 -0.003
-0.222 -0.003 -1.552
0.006 0.001 -0.001
-0.002 -0.004 0.001
-0.001 0.000 0.001

atensor 30 C
2.047 1.897 0.349
1.897 0.539 0.663
0.349 0.663 0.670
0.026 0.020 0.018
-0.028 0.026 -0.014
0.008 -0.003 0.071

atensor 31 H
2.036 1.388 0.589
1.388 -1.001 0.253
0.589 0.253 -1.416
0.019 0.002 0.006
0.011 0.002 0.003
-0.001 -0.001 -0.003

atensor 32 H
0.796 1.331 2.095
1.331 -1.158 0.993
2.095 0.993 -0.147
0.008 0.001 0.020
0.010 0.002 0.012
-0.002 -0.008 -0.007

atensor 33 H
-0.248 1.189 0.571
1.189 -0.301 0.532
0.571 0.532 -1.213
0.010 0.007 0.009
0.007 0.003 0.005
0.002 -0.002 -0.002

atensor 34 H
-1.390 2.872 -0.466
2.872 0.771 -0.610
-0.466 -0.610 -3.765
0.036 0.066 -0.006
0.013 -0.008 0.000
-0.003 -0.007 0.017

atensor 35 H
0.235 -0.259 -0.106
-0.259 -0.696 0.033
-0.106 0.033 -0.690
0.003 -0.002 0.000

-0.001 -0.002 0.000
0.000 0.000 0.001

atensor 36 H
0.337 -0.372 -0.055
-0.372 0.106 0.029
-0.055 0.029 -0.240
0.000 -0.002 0.000
-0.002 -0.001 0.000
0.000 0.000 0.000

atensor 37 H
-0.474 -0.629 -0.003
-0.629 0.530 0.013
-0.003 0.013 -0.759
-0.006 -0.005 0.001
-0.007 -0.001 0.001
0.001 0.001 0.000

atensor 38 Cr
17.763 2.563 -0.262
2.563 27.076 -0.869
-0.262 -0.869 16.849
0.181 -0.809 0.320
-0.825 0.724 0.191
0.321 0.189 2.303

atensor 39 Br
31.364 1.560 10.672
1.560 12.066 -26.335
10.672 -26.335 -28.686
-1.119 -0.250 -0.494
-0.229 -0.073 2.492
-0.812 1.945 3.016

atensor 40 Br
22.194 5.699 -24.961
5.699 17.050 20.947
-24.961 20.947 -24.480
-0.520 -0.583 1.516
-0.666 -0.492 -2.031
1.837 -1.493 2.838

orbtensor 1 N
-479.281 54.193 47.135
54.193 -548.298 17.272
47.135 17.272 -95.205
338.950 -3.912 -2.104
-3.912 349.532 -1.007
-2.104 -1.007 321.202

orbtensor 2 C
-272.176 26.129 24.527
26.129 -297.150 8.628
24.527 8.628 -73.148
252.700 5.872 -5.674
5.872 251.509 -2.895
-5.674 -2.895 211.609

orbtensor 3 C
-218.840 -44.958 23.581
-44.958 -287.439 18.083
23.581 18.083 -56.822
251.907 3.527 -3.929
3.527 262.827 -2.566
-3.929 -2.566 223.256

orbtensor 4 C
-299.347 -23.670 32.717
-23.670 -231.580 12.411
32.717 12.411 -57.951
256.820 3.289 -5.332
3.289 252.550 -2.319
-5.332 -2.319 217.260

orbtensor 5 C
-287.705 2.937 29.715
2.937 -275.558 11.275
29.715 11.275 -58.400
269.107 0.351 -4.438
0.351 266.574 -1.730
-4.438 -1.730 235.192

orbtensor 6 C
-274.267 20.946 21.576
20.946 -295.338 7.761
21.576 7.761 -100.045
263.029 -5.222 -5.644
-5.222 260.585 -1.639
-5.644 -1.639 217.536

orbtensor 7 C
-295.948 10.219 30.106
10.219 -208.949 6.725
30.106 6.725 -60.365
257.825 -4.261 -5.049
-4.261 251.200 -1.276
-5.049 -1.276 217.278

orbtensor 8 C
-250.135 55.071 23.052
55.071 -267.464 4.543
23.052 4.543 -50.322
253.524 -5.982 -4.040
-5.982 255.586 -1.135
-4.040 -1.135 220.032

orbtensor 9 C
-233.115 -33.883 24.689
-33.883 -291.370 16.815
24.689 16.815 -57.952
252.258 -3.871 -4.140
-3.871 257.197 -1.551
-4.140 -1.551 218.891

orbtensor 10 C
-300.853 -15.896 28.364
-15.896 -249.616 10.658
28.364 10.658 -89.723
269.558 -1.101 -4.369
-1.101 264.629 -1.421
-4.369 -1.421 235.565

orbtensor 11 C
-215.744 32.161 -0.363
32.161 -130.730 -8.038
-0.363 -8.038 -204.884
244.708 -9.330 -0.978
-9.330 239.946 0.840
-0.978 0.840 233.305

orbtensor 12 C
-198.056 18.023 0.264
18.023 -104.706 24.875

0.264	24.875	-233.062
240.641	-2.865	-4.611
-2.865	236.236	-7.096
-4.611	-7.096	242.356

orbtensor 13 C

-225.505	-9.616	13.739
-9.616	-93.147	13.957
13.739	13.957	-217.880
244.227	5.169	-1.508
5.169	233.499	-4.824
-1.508	-4.824	243.006

orbtensor 14 C

-200.663	9.022	-9.333
9.022	-111.682	-41.081
-9.333	-41.081	-223.467
243.012	-0.449	4.416
-0.449	237.825	7.874
4.416	7.874	238.396

orbtensor 15 C

-55.887	0.656	6.495
0.656	-46.626	3.063
6.495	3.063	-49.104
218.375	-0.791	2.847
-0.791	218.006	-4.437
2.847	-4.437	227.668

orbtensor 16 H

3.272	-0.645	0.015
-0.645	2.115	1.320
0.015	1.320	1.644
23.114	0.381	-0.259
0.381	29.431	-6.854
-0.259	-6.854	28.921

orbtensor 17 H

3.527	0.497	-2.080
0.497	3.542	2.370
-2.080	2.370	3.000
29.854	-0.400	0.643
-0.400	20.927	-2.462
0.643	-2.462	28.407

orbtensor 18 H

5.131	0.391	-0.151
0.391	3.452	2.285
-0.151	2.285	-1.150
21.019	-3.201	-0.403
-3.201	26.847	0.717
-0.403	0.717	29.887

orbtensor 19 C

-53.363	-0.598	-5.764
-0.598	-44.732	2.486
-5.764	2.486	-54.379
225.407	1.728	-6.938
1.728	218.455	-1.653
-6.938	-1.653	222.584

orbtensor 20 H

2.417	-0.595	1.036
-0.595	2.165	0.783
1.036	0.783	2.585
26.266	3.906	-3.914
3.906	29.148	-5.084

-3.914 -5.084 26.091

orbtensor 21 H

2.745 -1.622 2.707
-1.622 3.694 1.143
2.707 1.143 0.376
25.121 3.575 -3.023
3.575 25.224 2.652
-3.023 2.652 28.308

orbtensor 22 H

-0.719 -1.236 1.411
-1.236 3.061 1.230
1.411 1.230 3.804
33.255 -1.325 -0.769
-1.325 22.582 -1.396
-0.769 -1.396 25.503

orbtensor 23 C

-50.594 -0.774 4.927
-0.774 -45.354 -3.415
4.927 -3.415 -56.534
228.542 2.765 5.103
2.765 218.779 1.300
5.103 1.300 219.127

orbtensor 24 C

-58.613 -0.703 -3.936
-0.703 -47.286 -3.088
-3.936 -3.088 -45.726
217.568 0.310 -0.323
0.310 219.050 5.469
-0.323 5.469 227.432

orbtensor 25 H

3.187 -0.978 -0.295
-0.978 1.855 -1.132
-0.295 -1.132 1.987
23.552 2.162 1.336
2.162 30.821 6.312
1.336 6.312 27.093

orbtensor 26 H

4.814 -0.316 -1.337
-0.316 2.922 -2.719
-1.337 -2.719 -0.305
21.856 -3.068 2.836
-3.068 26.817 0.383
2.836 0.383 29.077

orbtensor 27 H

4.506 0.077 1.722
0.077 3.029 -2.501
1.722 -2.501 2.531
29.443 0.241 -0.976
0.241 21.526 3.229
-0.976 3.229 28.219

orbtensor 28 H

-5.457 -5.975 0.655
-5.975 -16.999 1.511
0.655 1.511 -2.956
32.075 4.802 -1.359
4.802 41.552 -1.567
-1.359 -1.567 23.675

orbtensor 29 H

-18.330	-3.029	2.300
-3.029	-3.552	0.491
2.300	0.491	-1.901
41.554	2.357	-2.727
2.357	30.543	-0.793
-2.727	-0.793	21.581

orbtensor 30 C

-231.320	-15.583	-8.442
-15.583	-97.080	-23.139
-8.442	-23.139	-208.107
244.712	6.428	0.313
6.428	234.449	4.205
0.313	4.205	241.556

orbtensor 31 H

-1.078	-1.565	0.039
-1.565	2.851	-0.742
0.039	-0.742	4.372
33.162	-0.917	-1.144
-0.917	22.938	1.947
-1.144	1.947	25.241

orbtensor 32 H

1.331	-2.182	-2.720
-2.182	3.473	-0.908
-2.720	-0.908	2.010
26.717	3.158	3.151
3.158	24.605	-3.206
3.151	-3.206	27.333

orbtensor 33 H

1.945	-0.860	-0.771
-0.860	2.027	-0.509
-0.771	-0.509	3.197
28.024	5.361	2.786
5.361	30.047	3.373
2.786	3.373	23.433

orbtensor 34 H

-8.516	4.227	0.728
4.227	-13.872	0.132
0.728	0.132	-1.182
35.495	-1.233	-1.913
-1.233	34.956	-0.627
-1.913	-0.627	20.304

orbtensor 35 H

-18.350	0.182	2.085
0.182	-3.315	0.048
2.085	0.048	-2.224
42.132	-0.344	-2.627
-0.344	30.316	-0.423
-2.627	-0.423	21.796

orbtensor 36 H

-8.514	7.941	0.250
7.941	-13.307	-0.488
0.250	-0.488	-3.295
34.389	-6.946	-1.061
-6.946	38.028	0.110
-1.061	0.110	23.364

orbtensor 37 H

-4.778	-4.832	0.662
-4.832	-16.721	1.414
0.662	1.414	-1.745

```

31.233    1.248    -1.274
1.248    40.303    -1.133
-1.274    -1.133    22.000

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orbtensor 38 Cr
-5086.458  406.347  -81.052
406.347 -3608.278  -154.448
-81.052 -154.448 -5535.483
1810.272   -0.430   0.294
-0.430 1811.483   0.105
0.294   0.105 1812.357

```

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orbtensor 39 Br
-862.313  -61.921  -1.700
-61.921 -1070.541  443.108
-1.700  443.108  -926.543
3090.320   -1.622  -3.292
-1.622 3096.312   7.776
-3.292   7.776 3099.372

```

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orbtensor 40 Br
-861.021  -168.382   8.723
-168.382 -1158.553  -389.141
8.723  -389.141  -839.913
3092.580   -3.016   5.510
-3.016 3094.777   -6.800
5.510   -6.800 3098.645

```

```

gtensor (ppt)
-0.154    0.005    0.000
0.005   -0.155    0.000
0.000    0.000   -0.153
13.944    8.045   -1.814
8.045   13.446   -1.575
-1.814   -1.575    3.383

```

```

zfstensor (cm-1)
-0.565808    0.544344    0.196612
0.544344   -0.150905   -0.117023
0.196612   -0.117023    0.716713

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-2.4253	-37.70000	4468.28904	-7.04339	4461.24565	4423.54565
2	C	3.5897	24.44800	-1900.75665	4.74170	-1896.01495	-1871.56695
3	C	-0.5973	58.29633	316.29268	-2.52521	313.76748	372.06381
4	C	1.2737	45.91733	-674.41649	5.71426	-668.70223	-622.78490
5	C	-1.0677	49.73667	565.33787	-1.18384	564.15403	613.89070
6	C	0.5123	23.83333	-271.28452	0.11965	-271.16486	-247.33153
7	C	0.2263	53.68033	-119.84527	0.98467	-118.86060	-65.18027
8	C	-0.3357	53.74033	177.73813	-0.68845	177.04968	230.79001
9	C	-0.7387	48.63633	391.12979	1.26792	392.39771	441.03404
10	C	0.6070	43.18667	-321.41126	-1.85395	-323.26521	-280.07854
11	C	-0.5513	55.53367	291.93532	0.76139	292.69671	348.23038
12	C	1.2767	61.13633	-676.00501	0.86319	-675.14182	-614.00549
13	C	1.1263	61.40000	-596.40233	-1.21969	-597.62202	-536.22202
14	C	1.2763	61.14033	-675.82851	0.01043	-675.81807	-614.67774
15	C	0.4763	170.81067	-252.22223	1.51897	-250.70327	-79.89260
16	H	0.8550	29.49900	-113.86313	0.33830	-113.52482	-84.02582
17	H	0.1597	29.75233	-21.26333	0.67676	-20.58657	9.16577
18	H	0.0107	28.39533	-1.42051	1.59457	0.17405	28.56939
19	C	0.3313	171.32400	-175.44360	-0.46764	-175.91124	-4.58724
20	H	-0.5837	29.55733	77.72879	-0.27679	77.45200	107.00933
21	H	-0.1697	28.48933	22.59506	0.15192	22.74699	51.23632
22	H	-0.1203	29.16200	16.02518	-0.85069	15.17450	44.33650

23	C	0.3317	171.32200	-175.62010	-0.46790	-176.08800	-4.76600
24	C	0.4760	170.80833	-252.04573	1.16683	-250.87890	-80.07057
25	H	0.8543	29.49833	-113.77435	0.19994	-113.57440	-84.07607
26	H	0.0110	28.39367	-1.46491	1.41304	-0.05186	28.34181
27	H	0.1600	29.75133	-21.30772	0.41273	-20.89499	8.85635
28	H	0.6060	23.96333	-80.70299	-0.48310	-81.18609	-57.22275
29	H	-1.2980	23.29833	172.85888	-0.33445	172.52443	195.82276
30	C	1.1263	61.40333	-596.40233	-1.40734	-597.80968	-536.40634
31	H	-0.1210	29.16200	16.11396	-0.82878	15.28518	44.44718
32	H	-0.1687	28.48967	22.46189	0.18064	22.64253	51.13220
33	H	-0.5837	29.55767	77.72879	-0.30203	77.42676	106.98443
34	H	-1.4463	22.39500	192.61291	-1.34295	191.26996	213.66496
35	H	-0.3830	23.45167	51.00535	-0.20832	50.79704	74.24871
36	H	0.0673	23.55500	-8.96700	-0.14971	-9.11671	14.43829
37	H	-0.2367	23.43067	31.51767	-0.15549	31.36218	54.79284
38	Cr	21.6320	-2932.03567	50863.85790	14.00381	50877.86171	47945.82604
39	Br	5.5227	2142.20233	-2925.45508	-60.76178	-2986.21686	-844.01453
40	Br	5.5300	2142.17167	-2929.33968	-73.11194	-3002.45162	-860.27995

=====
CrL2-STO-PBE0-No-ZFS

Temperature: 298

Spin: 1.5

atensor 1 N

-3.086 0.222 -0.265
0.222 -3.760 -0.097
-0.265 -0.097 -5.031
0.003 0.000 0.003
0.003 0.012 0.000
0.003 0.001 0.024

atensor 2 C

3.106 0.992 0.152
0.992 2.280 0.001
0.152 0.001 4.685
-0.036 -0.007 0.006
0.058 0.027 -0.009
0.002 0.000 0.004

atensor 3 C

0.026 0.211 -0.264
0.211 -0.525 -0.102
-0.264 -0.102 -1.913
0.003 -0.001 0.000
0.002 0.004 0.000
0.000 0.000 0.001

atensor 4 C

0.581 0.091 0.274
0.091 0.034 0.132
0.274 0.132 2.723
-0.001 0.005 0.000
-0.004 -0.012 0.001
0.000 0.000 0.000

atensor 5 C

-0.493 -0.096 -0.163
-0.096 -1.016 -0.029
-0.163 -0.029 -1.782
0.002 -0.002 0.000
0.001 0.004 0.000
0.000 0.000 0.002

atensor 6 C

1.499 -0.473 -0.078

-0.473 -0.770 0.137
-0.078 0.137 0.697
0.012 -0.006 -0.001
-0.019 -0.021 0.003
-0.001 0.002 0.000

atensor 7 C
0.307 -0.099 0.070
-0.099 0.007 0.055
0.070 0.055 0.805
0.001 0.001 0.000
-0.002 -0.004 0.001
0.000 0.000 0.000

atensor 8 C
-0.194 -0.161 -0.108
-0.161 -0.287 -0.022
-0.108 -0.022 -1.091
0.001 0.001 0.000
0.000 0.001 0.000
0.000 0.000 0.000

atensor 9 C
-1.057 -0.251 0.107
-0.251 -0.929 0.064
0.107 0.064 -0.344
-0.005 -0.008 0.001
0.001 0.002 0.000
0.001 0.001 0.000

atensor 10 C
1.534 -1.034 -0.207
-1.034 1.156 0.044
-0.207 0.044 -0.488
0.000 -0.003 0.001
-0.001 -0.007 0.001
0.001 0.001 0.004

atensor 11 C
-0.038 -1.582 0.023
-1.582 -2.965 0.332
0.023 0.332 -0.529
0.054 0.011 0.002
-0.021 -0.002 0.007
0.004 0.003 0.072

atensor 12 C
0.060 -0.736 0.119
-0.736 1.182 -2.217
0.119 -2.217 1.363
0.033 0.006 -0.014
-0.014 0.008 0.008
0.000 0.025 0.059

atensor 13 C
1.673 1.578 -0.852
1.578 -0.662 -1.007
-0.852 -1.007 1.032
0.038 0.008 -0.008
-0.029 0.024 0.025
0.006 0.015 0.080

atensor 14 C
0.088 -0.151 0.198
-0.151 1.659 2.300
0.198 2.300 0.858
0.038 0.002 0.019

-0.014 0.006 0.001
0.007 -0.021 0.057

atensor 15 C
-0.037 -0.242 0.318
-0.242 0.409 -0.812
0.318 -0.812 1.039
0.003 0.000 -0.006
-0.003 0.001 0.001
-0.001 0.007 0.002

atensor 16 H
-0.858 -0.220 0.240
-0.220 0.616 -1.438
0.240 -1.438 0.480
-0.006 0.002 -0.005
-0.004 0.001 -0.004
0.003 0.007 0.000

atensor 17 H
-0.230 -1.283 1.681
-1.283 -0.275 -1.788
1.681 -1.788 0.725
-0.007 -0.002 0.000
-0.006 -0.003 0.001
-0.004 0.012 -0.004

atensor 18 H
-2.060 -0.248 0.546
-0.248 -1.392 -1.835
0.546 -1.835 2.866
-0.011 -0.006 -0.007
-0.006 0.001 -0.007
0.004 0.017 -0.015

atensor 19 C
0.625 0.458 -0.617
0.457 0.222 -0.418
-0.617 -0.418 0.547
0.002 0.001 -0.001
-0.001 0.003 -0.002
0.001 0.005 0.006

atensor 20 H
-1.232 0.976 -0.827
0.976 -1.043 -0.909
-0.827 -0.909 -1.317
0.006 0.004 -0.009
0.002 0.003 -0.004
0.000 0.003 0.003

atensor 21 H
-0.522 0.860 -2.247
0.860 -1.719 -1.163
-2.247 -1.163 1.060
0.003 -0.002 -0.015
0.004 0.004 -0.011
0.008 0.012 -0.004

atensor 22 H
1.501 1.247 -1.534
1.247 -1.204 -0.638
-1.534 -0.638 -0.866
0.011 -0.002 -0.007
0.007 0.005 -0.005
0.002 0.003 0.004

atensor 23 C
0.906 0.607 0.456
0.607 0.298 0.292
0.456 0.292 0.191
0.002 0.000 0.002
0.000 0.003 0.002
0.000 -0.005 0.006

atensor 24 C
-0.123 -0.040 -0.024
-0.040 0.589 0.902
-0.024 0.902 0.944
0.005 -0.001 0.005
-0.003 0.000 0.000
0.000 -0.007 0.001

atensor 25 H
-0.894 0.137 0.082
0.137 0.916 1.407
0.082 1.407 0.215
-0.005 0.000 0.006
-0.003 0.001 0.004
-0.001 -0.008 0.000

atensor 26 H
-2.022 0.283 0.669
0.283 -0.962 2.241
0.669 2.241 2.397
-0.011 -0.009 0.007
-0.005 0.000 0.007
-0.005 -0.016 -0.015

atensor 27 H
-0.966 -0.929 -1.174
-0.929 0.142 2.176
-1.174 2.176 1.043
-0.005 -0.005 0.001
-0.006 -0.005 0.000
0.006 -0.011 -0.004

atensor 28 H
1.364 0.639 -0.218
0.639 0.435 -0.109
-0.218 -0.109 -0.042
0.005 0.001 0.000
0.005 0.005 -0.001
0.000 0.000 0.004

atensor 29 H
0.171 0.283 -0.195
0.283 -1.711 -0.011
-0.195 -0.011 -1.212
0.003 0.000 0.000
0.001 -0.001 0.000
0.000 0.000 0.002

atensor 30 C
1.999 1.866 0.391
1.865 -0.480 0.705
0.391 0.705 0.524
0.042 0.006 0.017
-0.033 0.021 -0.011
0.007 -0.010 0.080

atensor 31 H
2.061 1.481 0.613
1.481 -1.107 0.278

0.613 0.278 -1.525
0.012 -0.002 0.005
0.008 0.005 0.003
-0.004 -0.003 0.003

atensor 32 H
0.639 1.390 2.203
1.390 -1.478 1.081
2.203 1.081 -0.340
0.004 -0.004 0.013
0.006 0.003 0.009
-0.011 -0.012 -0.005

atensor 33 H
-0.866 1.240 0.568
1.240 -0.887 0.558
0.568 0.558 -1.839
0.008 0.004 0.007
0.003 0.003 0.003
-0.001 -0.005 0.001

atensor 34 H
-1.101 3.382 -0.526
3.382 1.244 -0.699
-0.526 -0.699 -3.719
0.027 0.038 -0.002
0.007 0.002 0.000
-0.001 -0.004 0.023

atensor 35 H
0.214 -0.237 -0.104
-0.237 -0.742 0.033
-0.104 0.033 -0.684
0.001 -0.001 0.000
0.001 -0.001 0.000
0.000 0.000 0.002

atensor 36 H
0.497 -0.308 -0.060
-0.308 0.233 0.022
-0.060 0.022 -0.092
0.000 -0.001 0.000
0.000 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.491 -0.674 0.001
-0.674 0.533 0.018
0.001 0.018 -0.761
-0.004 -0.002 0.001
-0.003 -0.002 0.001
0.001 0.000 0.002

atensor 38 Cr
26.577 2.905 -0.390
2.905 36.846 -1.009
-0.390 -1.009 24.828
1.080 -0.725 0.311
-0.910 1.224 0.221
0.320 0.197 3.160

atensor 39 Br
31.732 2.913 9.253
2.913 11.479 -28.609
9.253 -28.609 -23.336
-1.520 -0.253 -0.401
-0.375 -1.161 1.989

-0.492 1.236 1.078

atensor 40 Br

23.513 7.843 -22.746
7.843 16.957 23.304
-22.746 23.304 -20.574
-1.121 -0.449 1.053
-0.745 -1.462 -1.594
1.165 -0.895 0.980

orbtensor 1 N

-467.892 44.203 52.989
44.203 -536.022 20.720
52.989 20.720 -42.610
322.780 -4.642 -3.987
-4.642 332.541 -1.661
-3.987 -1.661 290.277

orbtensor 2 C

-288.056 28.719 25.335
28.719 -320.454 9.095
25.335 9.095 -81.288
259.852 6.432 -4.611
6.432 261.368 -2.660
-4.611 -2.660 227.161

orbtensor 3 C

-229.919 -39.700 25.911
-39.700 -277.394 17.354
25.911 17.354 -48.035
260.026 -1.695 -4.958
-1.695 254.950 -1.593
-4.958 -1.593 221.258

orbtensor 4 C

-304.491 -25.949 33.483
-25.949 -251.186 13.729
33.483 13.729 -58.336
252.800 2.460 -4.007
2.460 263.737 -2.485
-4.007 -2.485 223.105

orbtensor 5 C

-290.369 2.891 31.555
2.891 -270.728 11.652
31.555 11.652 -46.863
271.263 0.989 -5.360
0.989 261.433 -1.793
-5.360 -1.793 230.517

orbtensor 6 C

-284.482 14.512 22.829
14.512 -311.388 9.235
22.829 9.235 -103.622
270.021 0.481 -4.926
0.481 268.756 -2.011
-4.926 -2.011 232.420

orbtensor 7 C

-298.328 13.841 30.180
13.841 -221.309 6.888
30.180 6.888 -60.900
255.220 -5.663 -4.010
-5.663 261.290 -1.367
-4.010 -1.367 222.099

orbtensor 8 C

-260.848	46.561	24.888
46.561	-269.342	5.704
24.888	5.704	-50.572
259.941	2.635	-4.781
2.635	256.599	-2.070
-4.781	-2.070	224.339

orbtensor 9 C

-246.989	-32.216	26.364
-32.216	-293.383	16.679
26.364	16.679	-58.146
261.277	-7.178	-4.574
-7.178	256.121	-0.847
-4.574	-0.847	223.176

orbtensor 10 C

-300.665	-20.674	29.850
-20.674	-246.526	11.553
29.850	11.553	-80.306
267.828	1.455	-5.054
1.455	262.969	-1.977
-5.054	-1.977	229.652

orbtensor 11 C

-229.894	25.714	0.404
25.714	-115.330	-8.702
0.404	-8.702	-215.800
259.060	-2.496	-0.595
-2.496	231.749	1.458
-0.595	1.458	253.377

orbtensor 12 C

-213.541	20.677	0.277
20.677	-99.303	23.377
0.277	23.377	-239.018
261.975	-3.442	-4.865
-3.442	237.973	-2.061
-4.865	-2.061	256.179

orbtensor 13 C

-241.981	-4.511	10.573
-4.511	-87.706	11.731
10.573	11.731	-232.181
260.139	0.499	3.210
0.499	235.805	-0.830
3.210	-0.830	258.733

orbtensor 14 C

-215.601	11.949	-7.332
11.949	-106.086	-41.570
-7.332	-41.570	-230.051
264.042	-2.168	3.046
-2.168	238.669	4.507
3.046	4.507	253.410

orbtensor 15 C

-51.656	1.941	3.147
1.941	-41.609	2.532
3.147	2.532	-49.353
220.414	-1.781	5.087
-1.781	217.437	-3.488
5.087	-3.488	232.016

orbtensor 16 H

3.618	-0.787	-0.329
-0.787	2.493	1.565
-0.329	1.565	1.538

22.844	0.665	-0.053
0.665	29.448	-7.153
-0.053	-7.153	29.173

orbtensor 17 H

2.142	0.533	-2.766
0.533	3.256	2.117
-2.766	2.117	1.815
31.750	-0.620	1.228
-0.620	21.116	-1.999
1.228	-1.999	29.526

orbtensor 18 H

4.825	0.453	-0.639
0.453	3.936	1.387
-0.639	1.387	-2.976
21.558	-3.397	-0.301
-3.397	26.556	1.887
-0.301	1.887	31.534

orbtensor 19 C

-49.816	-1.021	-3.092
-1.021	-39.191	1.124
-3.092	1.124	-51.441
227.421	1.830	-8.896
1.830	217.381	0.077
-8.896	0.077	224.674

orbtensor 20 H

3.245	-0.880	1.492
-0.880	2.883	1.057
1.492	1.057	3.347
25.759	4.147	-4.458
4.147	29.091	-5.318
-4.458	-5.318	25.727

orbtensor 21 H

2.388	-1.259	3.372
-1.259	4.324	0.327
3.372	0.327	-1.191
25.601	3.050	-3.449
3.050	24.885	3.582
-3.449	3.582	30.009

orbtensor 22 H

-1.902	-0.895	2.030
-0.895	3.238	0.839
2.030	0.839	3.824
35.007	-1.733	-1.185
-1.733	22.365	-0.851
-1.185	-0.851	25.622

orbtensor 23 C

-48.369	-1.098	2.439
-1.098	-39.455	-2.143
2.439	-2.143	-52.540
231.523	2.663	6.875
2.663	217.374	-0.113
6.875	-0.113	220.586

orbtensor 24 C

-53.130	0.910	-2.249
0.910	-42.302	-3.527
-2.249	-3.527	-47.297
218.696	-1.001	-1.583
-1.001	218.373	5.399
-1.583	5.399	232.802

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orbtensor 25 H
3.653   -1.153   -0.077
-1.153   2.134   -1.370
-0.077  -1.370   1.787
23.206   2.500   1.244
2.500   30.895   6.555
1.244    6.555   27.365

orbtensor 26 H
4.636   -0.029   -1.311
-0.029   3.519   -2.148
-1.311   -2.148   -2.423
22.429   -3.517   3.078
-3.517   26.312   -0.477
3.078   -0.477   30.906

orbtensor 27 H
3.443    0.220    2.355
0.220    2.731   -2.385
2.355   -2.385    0.963
31.015   -0.140   -1.635
-0.140   21.638    2.966
-1.635    2.966   29.739

orbtensor 28 H
-4.014   -6.360    0.635
-6.360  -16.190    1.574
0.635    1.574   -1.862
30.730    5.144   -1.431
5.144   40.862   -1.668
-1.431   -1.668   21.922

orbtensor 29 H
-18.806  -3.971    2.284
-3.971   -2.868    0.516
2.284    0.516   -2.864
41.672    3.242   -2.792
3.242   29.967   -0.877
-2.792   -0.877   21.569

orbtensor 30 C
-246.251 -10.060   -5.715
-10.060  -91.625  -24.530
-5.715  -24.530 -224.045
258.465    0.659   -3.238
0.659  236.223    3.147
-3.238    3.147  259.992

orbtensor 31 H
-2.489   -1.184   -0.247
-1.184    3.048   -0.434
-0.247   -0.434   4.555
35.026   -1.424   -1.119
-1.424   22.622    1.557
-1.119    1.557   25.346

orbtensor 32 H
0.549   -1.756   -3.653
-1.756    4.242   -0.413
-3.653   -0.413    0.719
27.502    2.504    3.902
2.504   24.111   -3.766
3.902   -3.766   28.888

orbtensor 33 H
2.545   -1.232   -1.132

```

-1.232	2.656	-0.665
-1.132	-0.665	4.217
27.784	5.702	3.261
5.702	30.028	3.482
3.261	3.482	22.766

orbtensor 34 H

-7.228	6.645	0.491
6.645	-13.610	-0.171
0.491	-0.171	-0.641
34.494	-3.174	-1.825
-3.174	34.698	-0.424
-1.825	-0.424	19.171

orbtensor 35 H

-19.135	0.367	2.096
0.367	-2.498	-0.046
2.096	-0.046	-2.829
42.858	-0.532	-2.710
-0.532	29.651	-0.364
-2.710	-0.364	21.801

orbtensor 36 H

-7.812	8.407	0.203
8.407	-13.046	-0.538
0.203	-0.538	-2.780
33.801	-7.306	-1.109
-7.306	37.819	0.109
-1.109	0.109	22.257

orbtensor 37 H

-3.766	-5.895	0.655
-5.895	-17.027	1.594
0.655	1.594	-1.181
30.488	2.014	-1.360
2.014	40.602	-1.304
-1.360	-1.304	20.922

orbtensor 38 Cr

-5209.892	663.052	-144.382
663.052	-3451.346	-222.735
-144.382	-222.735	-6037.087
1803.939	0.419	0.080
0.419	1814.508	-0.566
0.080	-0.566	1804.759

orbtensor 39 Br

-401.295	-34.009	17.040
-34.009	-597.308	202.493
17.040	202.493	-486.547
3094.503	-1.238	-2.255
-1.238	3099.779	6.255
-2.255	6.255	3100.982

orbtensor 40 Br

-413.999	-84.345	-24.166
-84.345	-637.795	-171.386
-24.166	-171.386	-435.661
3096.079	-2.427	3.892
-2.427	3098.531	-5.599
3.892	-5.599	3100.652

gtensor (ppt)

-0.167	0.005	0.000
0.005	-0.150	-0.001
0.000	-0.001	-0.165
6.199	7.382	-2.165

7.382 5.167 -1.621
 -2.165 -1.621 -7.333

averaging

2H Average:34

4H Average:29

9,10H Average:16,17,18,20,21,22

5H Average:35

8,11H Average:25,26,27,31,32,33

6H Average:36

3H Average:28

7H Average:37

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.9460	-33.64200	7237.65728	-5.76873	7231.88855	7198.24655
2	C	3.3553	19.52767	-1768.80182	0.22909	-1768.57273	-1749.04507
3	C	-0.8013	60.29533	422.43191	-1.69638	420.73553	481.03086
4	C	1.1083	41.87633	-584.27042	1.84256	-582.42786	-540.55153
5	C	-1.0943	51.75100	576.89016	-0.75144	576.13872	627.88972
6	C	0.4723	23.90167	-248.99585	0.79293	-248.20292	-224.30125
7	C	0.3720	52.69067	-196.10400	0.65228	-195.45171	-142.76105
8	C	-0.5233	53.37233	275.88107	-0.49181	275.38926	328.76160
9	C	-0.7777	47.35200	409.95576	0.89047	410.84622	458.19822
10	C	0.7330	44.31733	-386.40922	-0.13015	-386.53937	-342.22204
11	C	-1.1360	61.05400	598.85522	2.80491	601.66012	662.71412
12	C	0.9017	68.08833	-475.32376	1.01845	-474.30530	-406.21697
13	C	0.7283	64.26967	-383.94913	-2.30224	-386.25138	-321.98171
14	C	0.9020	68.12767	-475.49948	1.01847	-474.48101	-406.35334
15	C	0.4723	175.74967	-248.99585	0.87434	-248.12151	-72.37184
16	H	0.0777	29.70467	-10.29729	0.12421	-10.17308	19.53159
17	H	0.0687	29.86833	-9.10404	0.63924	-8.46480	21.40353
18	H	-0.2037	28.47767	27.00275	0.88892	27.89168	56.36934
19	C	0.4683	176.34267	-246.88720	-0.86683	-247.75403	-71.41136
20	H	-1.1933	30.01733	158.21581	-0.49613	157.71968	187.73701
21	H	-0.3927	28.67200	52.06096	-0.17598	51.88497	80.55697
22	H	-0.1830	29.38467	24.26270	-0.82508	23.43762	52.82229
23	C	0.4687	176.37300	-247.06292	-0.86763	-247.93056	-71.55756
24	C	0.4720	175.71400	-248.82013	0.87361	-247.94652	-72.23252
25	H	0.0777	29.68000	-10.29729	0.12423	-10.17306	19.50694
26	H	-0.2043	28.45967	27.09114	0.88902	27.98016	56.43983
27	H	0.0683	29.84300	-9.05984	0.63930	-8.42054	21.42246
28	H	0.5903	23.81600	-78.26821	-0.42877	-78.69699	-54.88099
29	H	-0.9160	22.89000	121.44610	-0.21737	121.22873	144.11873
30	C	0.7287	64.25300	-384.12485	-2.30280	-386.42765	-322.17465
31	H	-0.1837	29.36933	24.35109	-0.82512	23.52597	52.89530
32	H	-0.3923	28.67033	52.01676	-0.17567	51.84109	80.51142
33	H	-1.1933	29.99867	158.21581	-0.49633	157.71948	187.71815
34	H	-1.1747	22.29467	155.74093	-1.90835	153.83258	176.12724
35	H	-0.4033	23.28267	53.47518	-0.02111	53.45407	76.73673
36	H	0.2127	23.41300	-28.19600	0.00618	-28.18982	-4.77682
37	H	-0.2410	23.34600	31.95252	0.08467	32.03719	55.38319
38	Cr	31.2383	-3091.70633	73125.96135	27.57492	73153.53626	70061.82993
39	Br	6.0907	2603.37133	-3212.03704	-40.98478	-3253.02182	-649.65049
40	Br	6.0977	2602.60233	-3215.72864	-40.99712	-3256.72576	-654.12342

=====
 CrL2-STO-PBE0-ORCA
 Temperature: 298
 Spin: 1.5

atensor 1 N
 -3.086 0.222 -0.265

0.222 -3.760 -0.097
-0.265 -0.097 -5.031
0.003 0.000 0.003
0.003 0.012 0.000
0.003 0.001 0.024

atensor 2 C
3.106 0.992 0.152
0.992 2.280 0.001
0.152 0.001 4.685
-0.036 -0.007 0.006
0.058 0.027 -0.009
0.002 0.000 0.004

atensor 3 C
0.026 0.211 -0.264
0.211 -0.525 -0.102
-0.264 -0.102 -1.913
0.003 -0.001 0.000
0.002 0.004 0.000
0.000 0.000 0.001

atensor 4 C
0.581 0.091 0.274
0.091 0.034 0.132
0.274 0.132 2.723
-0.001 0.005 0.000
-0.004 -0.012 0.001
0.000 0.000 0.000

atensor 5 C
-0.493 -0.096 -0.163
-0.096 -1.016 -0.029
-0.163 -0.029 -1.782
0.002 -0.002 0.000
0.001 0.004 0.000
0.000 0.000 0.002

atensor 6 C
1.499 -0.473 -0.078
-0.473 -0.770 0.137
-0.078 0.137 0.697
0.012 -0.006 -0.001
-0.019 -0.021 0.003
-0.001 0.002 0.000

atensor 7 C
0.307 -0.099 0.070
-0.099 0.007 0.055
0.070 0.055 0.805
0.001 0.001 0.000
-0.002 -0.004 0.001
0.000 0.000 0.000

atensor 8 C
-0.194 -0.161 -0.108
-0.161 -0.287 -0.022
-0.108 -0.022 -1.091
0.001 0.001 0.000
0.000 0.001 0.000
0.000 0.000 0.000

atensor 9 C
-1.057 -0.251 0.107
-0.251 -0.929 0.064
0.107 0.064 -0.344
-0.005 -0.008 0.001

0.001 0.002 0.000
0.001 0.001 0.000

atensor 10 C
1.534 -1.034 -0.207
-1.034 1.156 0.044
-0.207 0.044 -0.488
0.000 -0.003 0.001
-0.001 -0.007 0.001
0.001 0.001 0.004

atensor 11 C
-0.038 -1.582 0.023
-1.582 -2.965 0.332
0.023 0.332 -0.529
0.054 0.011 0.002
-0.021 -0.002 0.007
0.004 0.003 0.072

atensor 12 C
0.060 -0.736 0.119
-0.736 1.182 -2.217
0.119 -2.217 1.363
0.033 0.006 -0.014
-0.014 0.008 0.008
0.000 0.025 0.059

atensor 13 C
1.673 1.578 -0.852
1.578 -0.662 -1.007
-0.852 -1.007 1.032
0.038 0.008 -0.008
-0.029 0.024 0.025
0.006 0.015 0.080

atensor 14 C
0.088 -0.151 0.198
-0.151 1.659 2.300
0.198 2.300 0.858
0.038 0.002 0.019
-0.014 0.006 0.001
0.007 -0.021 0.057

atensor 15 C
-0.037 -0.242 0.318
-0.242 0.409 -0.812
0.318 -0.812 1.039
0.003 0.000 -0.006
-0.003 0.001 0.001
-0.001 0.007 0.002

atensor 16 H
-0.858 -0.220 0.240
-0.220 0.616 -1.438
0.240 -1.438 0.480
-0.006 0.002 -0.005
-0.004 0.001 -0.004
0.003 0.007 0.000

atensor 17 H
-0.230 -1.283 1.681
-1.283 -0.275 -1.788
1.681 -1.788 0.725
-0.007 -0.002 0.000
-0.006 -0.003 0.001
-0.004 0.012 -0.004

atensor 18 H
-2.060 -0.248 0.546
-0.248 -1.392 -1.835
0.546 -1.835 2.866
-0.011 -0.006 -0.007
-0.006 0.001 -0.007
0.004 0.017 -0.015

atensor 19 C
0.625 0.458 -0.617
0.457 0.222 -0.418
-0.617 -0.418 0.547
0.002 0.001 -0.001
-0.001 0.003 -0.002
0.001 0.005 0.006

atensor 20 H
-1.232 0.976 -0.827
0.976 -1.043 -0.909
-0.827 -0.909 -1.317
0.006 0.004 -0.009
0.002 0.003 -0.004
0.000 0.003 0.003

atensor 21 H
-0.522 0.860 -2.247
0.860 -1.719 -1.163
-2.247 -1.163 1.060
0.003 -0.002 -0.015
0.004 0.004 -0.011
0.008 0.012 -0.004

atensor 22 H
1.501 1.247 -1.534
1.247 -1.204 -0.638
-1.534 -0.638 -0.866
0.011 -0.002 -0.007
0.007 0.005 -0.005
0.002 0.003 0.004

atensor 23 C
0.906 0.607 0.456
0.607 0.298 0.292
0.456 0.292 0.191
0.002 0.000 0.002
0.000 0.003 0.002
0.000 -0.005 0.006

atensor 24 C
-0.123 -0.040 -0.024
-0.040 0.589 0.902
-0.024 0.902 0.944
0.005 -0.001 0.005
-0.003 0.000 0.000
0.000 -0.007 0.001

atensor 25 H
-0.894 0.137 0.082
0.137 0.916 1.407
0.082 1.407 0.215
-0.005 0.000 0.006
-0.003 0.001 0.004
-0.001 -0.008 0.000

atensor 26 H
-2.022 0.283 0.669
0.283 -0.962 2.241

0.669 2.241 2.397
-0.011 -0.009 0.007
-0.005 0.000 0.007
-0.005 -0.016 -0.015

atensor 27 H
-0.966 -0.929 -1.174
-0.929 0.142 2.176
-1.174 2.176 1.043
-0.005 -0.005 0.001
-0.006 -0.005 0.000
0.006 -0.011 -0.004

atensor 28 H
1.364 0.639 -0.218
0.639 0.435 -0.109
-0.218 -0.109 -0.042
0.005 0.001 0.000
0.005 0.005 -0.001
0.000 0.000 0.004

atensor 29 H
0.171 0.283 -0.195
0.283 -1.711 -0.011
-0.195 -0.011 -1.212
0.003 0.000 0.000
0.001 -0.001 0.000
0.000 0.000 0.002

atensor 30 C
1.999 1.866 0.391
1.865 -0.480 0.705
0.391 0.705 0.524
0.042 0.006 0.017
-0.033 0.021 -0.011
0.007 -0.010 0.080

atensor 31 H
2.061 1.481 0.613
1.481 -1.107 0.278
0.613 0.278 -1.525
0.012 -0.002 0.005
0.008 0.005 0.003
-0.004 -0.003 0.003

atensor 32 H
0.639 1.390 2.203
1.390 -1.478 1.081
2.203 1.081 -0.340
0.004 -0.004 0.013
0.006 0.003 0.009
-0.011 -0.012 -0.005

atensor 33 H
-0.866 1.240 0.568
1.240 -0.887 0.558
0.568 0.558 -1.839
0.008 0.004 0.007
0.003 0.003 0.003
-0.001 -0.005 0.001

atensor 34 H
-1.101 3.382 -0.526
3.382 1.244 -0.699
-0.526 -0.699 -3.719
0.027 0.038 -0.002
0.007 0.002 0.000

-0.001 -0.004 0.023

atensor 35 H
0.214 -0.237 -0.104
-0.237 -0.742 0.033
-0.104 0.033 -0.684
0.001 -0.001 0.000
0.001 -0.001 0.000
0.000 0.000 0.002

atensor 36 H
0.497 -0.308 -0.060
-0.308 0.233 0.022
-0.060 0.022 -0.092
0.000 -0.001 0.000
0.000 -0.001 0.000
0.000 0.000 0.001

atensor 37 H
-0.491 -0.674 0.001
-0.674 0.533 0.018
0.001 0.018 -0.761
-0.004 -0.002 0.001
-0.003 -0.002 0.001
0.001 0.000 0.002

atensor 38 Cr
26.577 2.905 -0.390
2.905 36.846 -1.009
-0.390 -1.009 24.828
1.080 -0.725 0.311
-0.910 1.224 0.221
0.320 0.197 3.160

atensor 39 Br
31.732 2.913 9.253
2.913 11.479 -28.609
9.253 -28.609 -23.336
-1.520 -0.253 -0.401
-0.375 -1.161 1.989
-0.492 1.236 1.078

atensor 40 Br
23.513 7.843 -22.746
7.843 16.957 23.304
-22.746 23.304 -20.574
-1.121 -0.449 1.053
-0.745 -1.462 -1.594
1.165 -0.895 0.980

orbtensor 1 N
-467.892 44.203 52.989
44.203 -536.022 20.720
52.989 20.720 -42.610
322.780 -4.642 -3.987
-4.642 332.541 -1.661
-3.987 -1.661 290.277

orbtensor 2 C
-288.056 28.719 25.335
28.719 -320.454 9.095
25.335 9.095 -81.288
259.852 6.432 -4.611
6.432 261.368 -2.660
-4.611 -2.660 227.161

orbtensor 3 C

-229.919	-39.700	25.911
-39.700	-277.394	17.354
25.911	17.354	-48.035
260.026	-1.695	-4.958
-1.695	254.950	-1.593
-4.958	-1.593	221.258

orbtensor 4 C

-304.491	-25.949	33.483
-25.949	-251.186	13.729
33.483	13.729	-58.336
252.800	2.460	-4.007
2.460	263.737	-2.485
-4.007	-2.485	223.105

orbtensor 5 C

-290.369	2.891	31.555
2.891	-270.728	11.652
31.555	11.652	-46.863
271.263	0.989	-5.360
0.989	261.433	-1.793
-5.360	-1.793	230.517

orbtensor 6 C

-284.482	14.512	22.829
14.512	-311.388	9.235
22.829	9.235	-103.622
270.021	0.481	-4.926
0.481	268.756	-2.011
-4.926	-2.011	232.420

orbtensor 7 C

-298.328	13.841	30.180
13.841	-221.309	6.888
30.180	6.888	-60.900
255.220	-5.663	-4.010
-5.663	261.290	-1.367
-4.010	-1.367	222.099

orbtensor 8 C

-260.848	46.561	24.888
46.561	-269.342	5.704
24.888	5.704	-50.572
259.941	2.635	-4.781
2.635	256.599	-2.070
-4.781	-2.070	224.339

orbtensor 9 C

-246.989	-32.216	26.364
-32.216	-293.383	16.679
26.364	16.679	-58.146
261.277	-7.178	-4.574
-7.178	256.121	-0.847
-4.574	-0.847	223.176

orbtensor 10 C

-300.665	-20.674	29.850
-20.674	-246.526	11.553
29.850	11.553	-80.306
267.828	1.455	-5.054
1.455	262.969	-1.977
-5.054	-1.977	229.652

orbtensor 11 C

-229.894	25.714	0.404
25.714	-115.330	-8.702
0.404	-8.702	-215.800

259.060	-2.496	-0.595
-2.496	231.749	1.458
-0.595	1.458	253.377

orbtensor 12 C

-213.541	20.677	0.277
20.677	-99.303	23.377
0.277	23.377	-239.018
261.975	-3.442	-4.865
-3.442	237.973	-2.061
-4.865	-2.061	256.179

orbtensor 13 C

-241.981	-4.511	10.573
-4.511	-87.706	11.731
10.573	11.731	-232.181
260.139	0.499	3.210
0.499	235.805	-0.830
3.210	-0.830	258.733

orbtensor 14 C

-215.601	11.949	-7.332
11.949	-106.086	-41.570
-7.332	-41.570	-230.051
264.042	-2.168	3.046
-2.168	238.669	4.507
3.046	4.507	253.410

orbtensor 15 C

-51.656	1.941	3.147
1.941	-41.609	2.532
3.147	2.532	-49.353
220.414	-1.781	5.087
-1.781	217.437	-3.488
5.087	-3.488	232.016

orbtensor 16 H

3.618	-0.787	-0.329
-0.787	2.493	1.565
-0.329	1.565	1.538
22.844	0.665	-0.053
0.665	29.448	-7.153
-0.053	-7.153	29.173

orbtensor 17 H

2.142	0.533	-2.766
0.533	3.256	2.117
-2.766	2.117	1.815
31.750	-0.620	1.228
-0.620	21.116	-1.999
1.228	-1.999	29.526

orbtensor 18 H

4.825	0.453	-0.639
0.453	3.936	1.387
-0.639	1.387	-2.976
21.558	-3.397	-0.301
-3.397	26.556	1.887
-0.301	1.887	31.534

orbtensor 19 C

-49.816	-1.021	-3.092
-1.021	-39.191	1.124
-3.092	1.124	-51.441
227.421	1.830	-8.896
1.830	217.381	0.077
-8.896	0.077	224.674


```

orbtensor 20 H
3.245   -0.880   1.492
-0.880   2.883   1.057
1.492   1.057   3.347
25.759   4.147  -4.458
4.147   29.091 -5.318
-4.458  -5.318   25.727

orbtensor 21 H
2.388   -1.259   3.372
-1.259   4.324   0.327
3.372   0.327  -1.191
25.601   3.050  -3.449
3.050   24.885  3.582
-3.449   3.582  30.009

orbtensor 22 H
-1.902   -0.895   2.030
-0.895   3.238   0.839
2.030   0.839   3.824
35.007  -1.733  -1.185
-1.733   22.365  -0.851
-1.185  -0.851   25.622

orbtensor 23 C
-48.369  -1.098   2.439
-1.098  -39.455  -2.143
2.439   -2.143 -52.540
231.523  2.663   6.875
2.663  217.374 -0.113
6.875   -0.113 220.586

orbtensor 24 C
-53.130  0.910   -2.249
0.910  -42.302  -3.527
-2.249  -3.527 -47.297
218.696  -1.001  -1.583
-1.001  218.373  5.399
-1.583   5.399 232.802

orbtensor 25 H
3.653   -1.153  -0.077
-1.153   2.134  -1.370
-0.077   -1.370  1.787
23.206   2.500   1.244
2.500   30.895   6.555
1.244   6.555   27.365

orbtensor 26 H
4.636   -0.029  -1.311
-0.029   3.519  -2.148
-1.311  -2.148  -2.423
22.429  -3.517   3.078
-3.517   26.312  -0.477
3.078   -0.477  30.906

orbtensor 27 H
3.443   0.220   2.355
0.220   2.731  -2.385
2.355  -2.385   0.963
31.015  -0.140  -1.635
-0.140  21.638   2.966
-1.635   2.966  29.739

orbtensor 28 H
-4.014  -6.360   0.635

```

-6.360	-16.190	1.574
0.635	1.574	-1.862
30.730	5.144	-1.431
5.144	40.862	-1.668
-1.431	-1.668	21.922

orbtensor 29 H

-18.806	-3.971	2.284
-3.971	-2.868	0.516
2.284	0.516	-2.864
41.672	3.242	-2.792
3.242	29.967	-0.877
-2.792	-0.877	21.569

orbtensor 30 C

-246.251	-10.060	-5.715
-10.060	-91.625	-24.530
-5.715	-24.530	-224.045
258.465	0.659	-3.238
0.659	236.223	3.147
-3.238	3.147	259.992

orbtensor 31 H

-2.489	-1.184	-0.247
-1.184	3.048	-0.434
-0.247	-0.434	4.555
35.026	-1.424	-1.119
-1.424	22.622	1.557
-1.119	1.557	25.346

orbtensor 32 H

0.549	-1.756	-3.653
-1.756	4.242	-0.413
-3.653	-0.413	0.719
27.502	2.504	3.902
2.504	24.111	-3.766
3.902	-3.766	28.888

orbtensor 33 H

2.545	-1.232	-1.132
-1.232	2.656	-0.665
-1.132	-0.665	4.217
27.784	5.702	3.261
5.702	30.028	3.482
3.261	3.482	22.766

orbtensor 34 H

-7.228	6.645	0.491
6.645	-13.610	-0.171
0.491	-0.171	-0.641
34.494	-3.174	-1.825
-3.174	34.698	-0.424
-1.825	-0.424	19.171

orbtensor 35 H

-19.135	0.367	2.096
0.367	-2.498	-0.046
2.096	-0.046	-2.829
42.858	-0.532	-2.710
-0.532	29.651	-0.364
-2.710	-0.364	21.801

orbtensor 36 H

-7.812	8.407	0.203
8.407	-13.046	-0.538
0.203	-0.538	-2.780
33.801	-7.306	-1.109

-7.306 37.819 0.109
 -1.109 0.109 22.257

orbtensor 37 H
 -3.766 -5.895 0.655
 -5.895 -17.027 1.594
 0.655 1.594 -1.181
 30.488 2.014 -1.360
 2.014 40.602 -1.304
 -1.360 -1.304 20.922

orbtensor 38 Cr
 -5209.892 663.052 -144.382
 663.052 -3451.346 -222.735
 -144.382 -222.735 -6037.087
 1803.939 0.419 0.080
 0.419 1814.508 -0.566
 0.080 -0.566 1804.759

orbtensor 39 Br
 -401.295 -34.009 17.040
 -34.009 -597.308 202.493
 17.040 202.493 -486.547
 3094.503 -1.238 -2.255
 -1.238 3099.779 6.255
 -2.255 6.255 3100.982

orbtensor 40 Br
 -413.999 -84.345 -24.166
 -84.345 -637.795 -171.386
 -24.166 -171.386 -435.661
 3096.079 -2.427 3.892
 -2.427 3098.531 -5.599
 3.892 -5.599 3100.652

gtensor (ppt)
 -0.167 0.005 0.000
 0.005 -0.150 -0.001
 0.000 -0.001 -0.165
 6.199 7.382 -2.165
 7.382 5.167 -1.621
 -2.165 -1.621 -7.333

zfstensor (cm-1)
 -11.272612 -0.465347 0.502707
 -0.465347 -9.245184 0.152960
 0.502707 0.152960 -9.197082

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	N	-3.9460	-33.64200	7237.79537	-13.92988	7223.86549	7190.22349
2	C	3.3553	19.52767	-1768.83557	0.06948	-1768.76609	-1749.23843
3	C	-0.8013	60.29533	422.43997	-3.96899	418.47098	478.76631
4	C	1.1083	41.87633	-584.28157	3.24448	-581.03709	-539.16075
5	C	-1.0943	51.75100	576.90117	-2.11523	574.78594	626.53694
6	C	0.4723	23.90167	-249.00060	-0.92059	-249.92119	-226.01952
7	C	0.3720	52.69067	-196.10774	0.98836	-195.11938	-142.42871
8	C	-0.5233	53.37233	275.88634	-1.16583	274.72050	328.09284
9	C	-0.7777	47.35200	409.96358	1.87182	411.83540	459.18740
10	C	0.7330	44.31733	-386.41659	-1.05304	-387.46963	-343.15230
11	C	-1.1360	61.05400	598.86664	2.09646	600.96311	662.01711
12	C	0.9017	68.08833	-475.33283	2.84798	-472.48485	-404.39652
13	C	0.7283	64.26967	-383.95646	-6.99317	-390.94963	-326.67996
14	C	0.9020	68.12767	-475.50855	3.70570	-471.80285	-403.67519
15	C	0.4723	175.74967	-249.00060	2.24976	-246.75084	-71.00117

16	H	0.0777	29.70467	-10.29748	0.62055	-9.67694	20.02773
17	H	0.0687	29.86833	-9.10421	1.40678	-7.69743	22.17090
18	H	-0.2037	28.47767	27.00327	1.95316	28.95643	57.43410
19	C	0.4683	176.34267	-246.89191	-2.38918	-249.28110	-72.93843
20	H	-1.1933	30.01733	158.21883	-1.00075	157.21807	187.23541
21	H	-0.3927	28.67200	52.06195	-0.97095	51.09100	79.76300
22	H	-0.1830	29.38467	24.26317	-2.46036	21.80280	51.18747
23	C	0.4687	176.37300	-247.06764	-1.80858	-248.87622	-72.50322
24	C	0.4720	175.71400	-248.82487	2.41465	-246.41023	-70.69623
25	H	0.0777	29.68000	-10.29748	0.73372	-9.56376	20.11624
26	H	-0.2043	28.45967	27.09166	2.15253	29.24419	57.70385
27	H	0.0683	29.84300	-9.06002	1.28422	-7.77579	22.06721
28	H	0.5903	23.81600	-78.26971	-1.05981	-79.32951	-55.51351
29	H	-0.9160	22.89000	121.44842	-0.90700	120.54142	143.43142
30	C	0.7287	64.25300	-384.13218	-6.15850	-390.29068	-326.03768
31	H	-0.1837	29.36933	24.35156	-2.19058	22.16098	51.53031
32	H	-0.3923	28.67033	52.01775	-0.39466	51.62310	80.29343
33	H	-1.1933	29.99867	158.21883	-0.78537	157.43346	187.43212
34	H	-1.1747	22.29467	155.74390	-2.99647	152.74743	175.04209
35	H	-0.4033	23.28267	53.47620	-0.31349	53.16270	76.44537
36	H	0.2127	23.41300	-28.19654	-0.08508	-28.28162	-4.86862
37	H	-0.2410	23.34600	31.95313	0.37496	32.32809	55.67409
38	Cr	31.2383	-3091.70633	73127.35662	5.60755	73132.96417	70041.25784
39	Br	6.0907	2603.37133	-3212.09833	-94.09828	-3306.19661	-702.82528
40	Br	6.0977	2602.60233	-3215.78999	-98.08468	-3313.87467	-711.27234

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FeL5-saddled-LS-STO-PBE0-Full-Finite

Temperature: 303

Spin: 1.5

atensor 1 C

-0.630 0.186 -0.043
0.186 -0.290 0.319
-0.043 0.319 -0.349
-0.033 -0.005 -0.001
0.009 0.011 0.002
-0.003 0.000 -0.001

atensor 2 C

-0.630 -0.186 -0.043
-0.186 -0.290 -0.319
-0.043 -0.319 -0.349
-0.033 0.005 -0.001
-0.009 0.011 -0.002
-0.003 0.000 -0.001

atensor 3 C

-0.630 -0.186 0.043
-0.186 -0.290 0.319
0.043 0.319 -0.349
-0.033 0.005 0.001
-0.009 0.011 0.002
0.003 0.000 -0.001

atensor 4 C

-0.630 0.186 0.043
0.186 -0.290 -0.319
0.043 -0.319 -0.349
-0.033 -0.005 0.001
0.009 0.011 -0.002
0.003 0.000 -0.001

atensor 5 C

-1.576 0.460 0.220
0.460 -0.512 0.513

0.220 0.513 -1.568
-0.016 0.016 0.007
0.035 0.002 0.006
0.004 0.001 -0.001

atensor 6 C
-1.576 -0.460 0.220
-0.460 -0.512 -0.513
0.220 -0.513 -1.568
-0.016 -0.016 0.007
-0.035 0.002 -0.006
0.004 -0.001 -0.001

atensor 7 C
-1.576 -0.460 -0.220
-0.460 -0.512 0.513
-0.220 0.513 -1.568
-0.016 -0.016 -0.007
-0.035 0.002 0.006
-0.004 0.001 -0.001

atensor 8 C
-1.576 0.460 -0.220
0.460 -0.512 -0.513
-0.220 -0.513 -1.568
-0.016 0.016 -0.007
0.035 0.002 -0.006
-0.004 -0.001 -0.001

atensor 9 C
0.464 0.671 0.327
0.671 0.454 0.011
0.327 0.011 0.447
0.004 0.008 0.002
0.004 0.003 0.002
0.003 0.002 -0.003

atensor 10 C
0.464 -0.671 0.327
-0.671 0.454 -0.011
0.327 -0.011 0.447
0.004 -0.008 0.002
-0.004 0.003 -0.002
0.003 -0.002 -0.003

atensor 11 C
0.464 -0.671 -0.327
-0.671 0.454 0.011
-0.327 0.011 0.447
0.004 -0.008 -0.002
-0.004 0.003 0.002
-0.003 0.002 -0.003

atensor 12 C
0.464 0.671 -0.327
0.671 0.454 -0.011
-0.327 -0.011 0.447
0.004 0.008 -0.002
0.004 0.003 -0.002
-0.003 -0.002 -0.003

atensor 13 C
-0.268 0.451 0.427
0.451 -1.377 0.149
0.427 0.149 -1.366
0.008 0.028 0.007
0.011 -0.005 0.004

0.002 -0.002 -0.002

atensor 14 C
-0.268 -0.451 0.427
-0.451 -1.377 -0.149
0.427 -0.149 -1.366
0.008 -0.028 0.007
-0.011 -0.005 -0.004
0.002 0.002 -0.002

atensor 15 C
-0.268 -0.451 -0.427
-0.451 -1.377 0.149
-0.427 0.149 -1.366
0.008 -0.028 -0.007
-0.011 -0.005 0.004
-0.002 -0.002 -0.002

atensor 16 C
-0.268 0.451 -0.427
0.451 -1.377 -0.149
-0.427 -0.149 -1.366
0.008 0.028 -0.007
0.011 -0.005 -0.004
-0.002 0.002 -0.002

atensor 17 C
-0.020 0.240 0.051
0.240 -0.017 0.023
0.051 0.023 -0.236
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.002

atensor 18 C
-0.020 -0.240 0.051
-0.240 -0.017 -0.023
0.051 -0.023 -0.236
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.002

atensor 19 C
-0.020 -0.240 -0.051
-0.240 -0.017 0.023
-0.051 0.023 -0.236
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 20 C
-0.020 0.240 -0.051
0.240 -0.017 -0.023
-0.051 -0.023 -0.236
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 23 C
0.162 -0.136 0.021
-0.136 0.257 -0.009
0.021 -0.009 0.045
0.000 -0.003 0.000
-0.003 0.002 -0.001
0.000 0.000 -0.001

atensor 24 C

0.162 0.136 0.021
0.136 0.257 0.009
0.021 0.009 0.045
0.000 0.003 0.000
0.003 0.002 0.001
0.000 0.000 -0.001

atensor 25 C
-0.363 0.162 0.313
0.162 -0.820 -0.033
0.313 -0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 0.001
0.002 0.003 -0.002

atensor 26 C
-0.363 -0.162 0.313
-0.162 -0.821 0.033
0.313 0.033 -0.742
0.010 -0.005 0.000
0.001 -0.029 -0.001
0.002 -0.003 -0.002

atensor 27 C
-0.363 -0.162 -0.313
-0.162 -0.820 -0.033
-0.313 -0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 0.001
-0.002 0.003 -0.002

atensor 28 C
-0.363 0.162 -0.313
0.162 -0.820 0.033
-0.313 0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 -0.001
-0.002 -0.003 -0.002

atensor 29 C
0.220 0.108 0.044
0.108 0.140 0.051
0.044 0.051 0.058
0.001 0.002 0.001
0.003 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.220 -0.108 0.044
-0.108 0.140 -0.051
0.044 -0.051 0.058
0.001 -0.002 0.001
-0.003 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.220 -0.108 -0.044
-0.108 0.140 0.051
-0.044 0.051 0.058
0.001 -0.002 -0.001
-0.003 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.220 0.108 -0.044
0.108 0.140 -0.051
-0.044 -0.051 0.058

0.001 0.002 -0.001
0.003 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.008 0.091 0.001
0.091 0.034 -0.015
0.001 -0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 34 C
0.008 -0.091 0.001
-0.091 0.034 0.015
0.001 0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 35 C
0.008 -0.091 -0.001
-0.091 0.034 -0.015
-0.001 -0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 36 C
0.008 0.091 -0.001
0.091 0.034 0.015
-0.001 0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.368 -17.100 -1.598
-17.100 -306.210 -34.163
-1.598 -34.163 -81.636
261.881 -3.875 -0.979
-3.875 258.313 4.204
-0.979 4.204 222.714

orbtensor 2 C
-220.368 17.100 -1.598
17.100 -306.210 34.163
-1.598 34.163 -81.636
261.881 3.875 -0.979
3.875 258.313 -4.204
-0.979 -4.204 222.714

orbtensor 3 C
-220.368 17.100 1.598
17.100 -306.210 -34.163
1.598 -34.163 -81.636
261.881 3.875 0.979
3.875 258.313 4.204
0.979 4.204 222.714

orbtensor 4 C
-220.368 -17.100 1.598
-17.100 -306.210 34.163
1.598 34.163 -81.636
261.881 -3.875 0.979
-3.875 258.313 -4.204
0.979 -4.204 222.714

orbtensor 5 C
-276.212 -12.908 2.770
-12.908 -296.076 -24.658
2.770 -24.658 -94.207
271.043 2.198 -0.318
2.198 265.976 3.256
-0.318 3.256 228.998

orbtensor 6 C
-276.212 12.908 2.770
12.908 -296.076 24.658
2.770 24.658 -94.207
271.043 -2.198 -0.318
-2.198 265.976 -3.256
-0.318 -3.256 228.998

orbtensor 7 C
-276.212 12.908 -2.770
12.908 -296.076 -24.658
-2.770 -24.658 -94.207
271.043 -2.198 0.318
-2.198 265.976 3.256
0.318 3.256 228.998

orbtensor 8 C
-276.212 -12.909 -2.770
-12.909 -296.076 24.658
-2.770 24.658 -94.207
271.043 2.198 0.318
2.198 265.976 -3.256
0.318 -3.256 228.998

orbtensor 9 C
-251.304 -17.109 8.657
-17.109 -253.695 -10.888
8.657 -10.888 -64.805
262.703 0.702 -0.479
0.702 262.933 0.846
-0.479 0.846 217.246

orbtensor 10 C
-251.304 17.109 8.657
17.109 -253.695 10.888
8.657 10.888 -64.805
262.703 -0.702 -0.479
-0.702 262.933 -0.846
-0.479 -0.846 217.246

orbtensor 11 C
-251.304 17.109 -8.657
17.109 -253.695 -10.888
-8.657 -10.888 -64.805
262.703 -0.702 0.479
-0.702 262.933 0.846
0.479 0.846 217.246

orbtensor 12 C
-251.304 -17.109 -8.657
-17.109 -253.695 10.888
-8.657 10.888 -64.805
262.703 0.702 0.479
0.702 262.933 -0.846
0.479 -0.846 217.246

orbtensor 13 C
-291.184 -7.658 29.280

-7.658	-281.792	-13.099
29.280	-13.099	-84.765
266.519	1.965	-1.564
1.965	270.756	0.788
-1.564	0.788	229.036

orbtensor 14 C

-291.184	7.658	29.280
7.658	-281.792	13.099
29.280	13.099	-84.765
266.519	-1.964	-1.564
-1.964	270.756	-0.788
-1.564	-0.788	229.035

orbtensor 15 C

-291.185	7.658	-29.280
7.658	-281.792	-13.099
-29.280	-13.099	-84.765
266.519	-1.965	1.564
-1.965	270.756	0.788
1.564	0.788	229.036

orbtensor 16 C

-291.185	-7.658	-29.280
-7.658	-281.792	13.099
-29.280	13.099	-84.765
266.519	1.964	1.564
1.964	270.756	-0.788
1.564	-0.788	229.035

orbtensor 17 C

-220.617	-107.808	-56.417
-107.808	-218.956	58.673
-56.417	58.673	-210.882
253.914	14.332	9.925
14.332	253.939	-9.934
9.925	-9.934	249.834

orbtensor 18 C

-220.618	107.808	-56.417
107.808	-218.956	-58.673
-56.417	-58.673	-210.881
253.914	-14.332	9.926
-14.332	253.939	9.934
9.926	9.934	249.834

orbtensor 19 C

-220.618	107.808	56.417
107.808	-218.956	58.673
56.417	58.673	-210.882
253.914	-14.332	-9.925
-14.332	253.939	-9.934
-9.925	-9.934	249.834

orbtensor 20 C

-220.618	-107.808	56.417
-107.808	-218.956	-58.673
56.417	-58.673	-210.882
253.914	14.332	-9.926
14.332	253.939	9.934
-9.926	9.934	249.834

orbtensor 23 C

-199.899	69.717	90.781
69.717	-165.664	49.438
90.781	49.438	-256.373
246.830	-14.814	-6.166

-14.814 250.046 -13.241
-6.166 -13.241 249.107

orbtensor 24 C
-199.899 -69.717 90.781
-69.717 -165.664 -49.438
90.781 -49.438 -256.373
246.830 14.814 -6.166
14.814 250.046 13.241
-6.166 13.241 249.107

orbtensor 25 C
-300.040 -14.281 35.998
-14.281 -218.667 12.304
35.998 12.304 -81.318
258.970 -4.022 -3.577
-4.022 261.080 1.056
-3.577 1.056 222.061

orbtensor 26 C
-300.040 14.281 35.998
14.281 -218.667 -12.304
35.998 -12.304 -81.318
258.970 4.022 -3.577
4.022 261.080 -1.056
-3.577 -1.056 222.061

orbtensor 27 C
-300.040 14.281 -35.998
14.281 -218.667 12.304
-35.998 12.304 -81.318
258.970 4.022 3.577
4.022 261.080 1.056
3.577 1.056 222.061

orbtensor 28 C
-300.040 -14.281 -35.998
-14.281 -218.667 -12.304
-35.998 -12.304 -81.318
258.970 -4.022 3.577
-4.022 261.080 -1.056
3.577 -1.056 222.061

orbtensor 29 C
-164.840 -67.454 -50.879
-67.454 -194.765 89.528
-50.879 89.528 -257.250
249.711 14.880 13.261
14.880 246.379 -6.422
13.261 -6.422 248.719

orbtensor 30 C
-164.840 67.454 -50.879
67.454 -194.765 -89.528
-50.879 -89.528 -257.250
249.711 -14.880 13.261
-14.880 246.379 6.422
13.261 6.422 248.719

orbtensor 31 C
-164.840 67.454 50.879
67.454 -194.765 89.528
50.879 89.528 -257.250
249.711 -14.880 -13.261
-14.880 246.379 -6.422
-13.261 -6.422 248.719

```

orbtensor 32 C
-164.840  -67.454   50.879
-67.454  -194.765  -89.528
50.879   -89.528 -257.250
249.711   14.880  -13.261
14.880   246.379   6.422
-13.261    6.422  248.719

```

```

orbtensor 33 C
-153.807  -70.075  -47.682
-70.075  -193.288   99.288
-47.682   99.288 -227.224
246.005   15.535   10.652
15.535   243.791  -9.554
10.652   -9.554  245.192

```

```

orbtensor 34 C
-153.807   70.075  -47.682
70.075  -193.288  -99.288
-47.682  -99.288 -227.223
246.005  -15.535   10.652
-15.535  243.791   9.554
10.652    9.554  245.192

```

```

orbtensor 35 C
-153.807   70.075   47.682
70.075  -193.288   99.288
47.682   99.288 -227.224
246.005  -15.535  -10.652
-15.535  243.791  -9.554
-10.652  -9.554  245.192

```

```

orbtensor 36 C
-153.807  -70.075   47.682
-70.075  -193.288  -99.288
47.682  -99.288 -227.223
246.005   15.535  -10.652
15.535   243.791   9.554
-10.652    9.554  245.192

```

```

gtensor (ppt)
-0.155   0.000   0.000
0.000  -0.154   0.000
0.000   0.000  -0.239
39.011   0.000   0.000
0.000  41.659   0.000
0.000   0.000  21.064

```

```

zfstensor (cm-1)
1.964053   0.000010   0.000321
0.000010   1.840828  -0.000123
0.000321  -0.000123  -73.369452

```

```

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4307	44.89800	223.02581	-6.07963	216.94617	261.84417
2	C	-0.4307	44.89800	223.02581	-6.07948	216.94633	261.84433
3	C	-0.4307	44.89800	223.02581	-6.07958	216.94622	261.84422
4	C	-0.4307	44.89800	223.02581	-6.07942	216.94639	261.84439
5	C	-1.2237	33.17400	633.69020	25.62263	659.31283	692.48683
6	C	-1.2237	33.17400	633.69020	25.62287	659.31307	692.48707

7	C	-1.2237	33.17400	633.69020	25.62232	659.31252	692.48652
8	C	-1.2237	33.17400	633.69020	25.62259	659.31279	692.48679
9	C	0.4563	57.69267	-236.31759	0.92267	-235.39492	-177.70226
10	C	0.4563	57.69267	-236.31759	0.92265	-235.39494	-177.70227
11	C	0.4563	57.69267	-236.31759	0.92222	-235.39537	-177.70271
12	C	0.4563	57.69267	-236.31759	0.92225	-235.39535	-177.70268
13	C	-1.0033	36.19000	519.58799	27.39279	546.98078	583.17078
14	C	-1.0033	36.18967	519.58799	27.39285	546.98084	583.17051
15	C	-1.0033	36.18967	519.58799	27.39222	546.98020	583.16987
16	C	-1.0033	36.18933	519.58799	27.39231	546.98029	583.16963
17	C	-0.0903	35.74400	46.78018	11.02451	57.80469	93.54869
18	C	-0.0903	35.74400	46.78018	11.02451	57.80469	93.54869
19	C	-0.0903	35.74367	46.78018	11.02443	57.80461	93.54828
20	C	-0.0903	35.74367	46.78018	11.02445	57.80463	93.54830
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1550	41.34900	-80.26858	8.27300	-71.99557	-30.64657
24	C	0.1550	41.34900	-80.26858	8.27300	-71.99557	-30.64657
25	C	-0.6483	47.36200	335.74705	7.14159	342.88864	390.25064
26	C	-0.6490	47.36200	336.09230	7.16660	343.25890	390.62090
27	C	-0.6483	47.36200	335.74705	7.14117	342.88823	390.25023
28	C	-0.6483	47.36200	335.74705	7.14116	342.88822	390.25022
29	C	0.1393	42.65133	-72.15541	6.15910	-65.99631	-23.34498
30	C	0.1393	42.65133	-72.15541	6.15912	-65.99629	-23.34496
31	C	0.1393	42.65133	-72.15541	6.15903	-65.99637	-23.34504
32	C	0.1393	42.65133	-72.15541	6.15906	-65.99634	-23.34501
33	C	-0.0050	53.55633	2.58931	3.95303	6.54234	60.09867
34	C	-0.0050	53.55667	2.58931	3.95302	6.54233	60.09900
35	C	-0.0050	53.55633	2.58931	3.95303	6.54234	60.09867
36	C	-0.0050	53.55667	2.58931	3.95302	6.54233	60.09900
A Average		-1.1135	34.68183	576.63909	26.50757	603.14666	637.82850
B Average		-0.5396	46.13000	279.42959	0.53405	279.96364	326.09364
M Average		0.4563	57.69267	-236.31759	0.92245	-235.39515	-177.70248

=====

FeL5-saddled-LS-STO-PBE0-Full-ORCA

Temperature: 303

Spin: 1.5

atensor 1 C

-0.630 0.186 -0.043
0.186 -0.290 0.319
-0.043 0.319 -0.349
-0.033 -0.005 -0.001
0.009 0.011 0.002
-0.003 0.000 -0.001

atensor 2 C

-0.630 -0.186 -0.043
-0.186 -0.290 -0.319
-0.043 -0.319 -0.349
-0.033 0.005 -0.001
-0.009 0.011 -0.002
-0.003 0.000 -0.001

atensor 3 C

-0.630 -0.186 0.043
-0.186 -0.290 0.319
0.043 0.319 -0.349
-0.033 0.005 0.001
-0.009 0.011 0.002
0.003 0.000 -0.001

atensor 4 C

-0.630 0.186 0.043
0.186 -0.290 -0.319

0.043 -0.319 -0.349
-0.033 -0.005 0.001
0.009 0.011 -0.002
0.003 0.000 -0.001

atensor 5 C
-1.576 0.460 0.220
0.460 -0.512 0.514
0.220 0.514 -1.568
-0.016 0.016 0.007
0.035 0.002 0.006
0.004 0.001 -0.001

atensor 6 C
-1.576 -0.460 0.220
-0.460 -0.512 -0.514
0.220 -0.514 -1.568
-0.016 -0.016 0.007
-0.035 0.002 -0.006
0.004 -0.001 -0.001

atensor 7 C
-1.576 -0.460 -0.220
-0.460 -0.512 0.514
-0.220 0.514 -1.568
-0.016 -0.016 -0.007
-0.035 0.002 0.006
-0.004 0.001 -0.001

atensor 8 C
-1.576 0.460 -0.220
0.460 -0.512 -0.514
-0.220 -0.514 -1.568
-0.016 0.016 -0.007
0.035 0.002 -0.006
-0.004 -0.001 -0.001

atensor 9 C
0.464 0.671 0.328
0.671 0.455 0.011
0.328 0.011 0.448
0.004 0.008 0.002
0.004 0.003 0.002
0.003 0.002 -0.003

atensor 10 C
0.464 -0.671 0.328
-0.671 0.455 -0.011
0.328 -0.011 0.448
0.004 -0.008 0.002
-0.004 0.003 -0.002
0.003 -0.002 -0.003

atensor 11 C
0.464 -0.671 -0.328
-0.671 0.455 0.011
-0.328 0.011 0.448
0.004 -0.008 -0.002
-0.004 0.003 0.002
-0.003 0.002 -0.003

atensor 12 C
0.464 0.671 -0.328
0.671 0.455 -0.011
-0.328 -0.011 0.448
0.004 0.008 -0.002
0.004 0.003 -0.002

-0.003 -0.002 -0.003

atensor 13 C
-0.268 0.451 0.427
0.451 -1.377 0.149
0.427 0.149 -1.366
0.008 0.028 0.007
0.011 -0.005 0.004
0.002 -0.002 -0.002

atensor 14 C
-0.268 -0.451 0.427
-0.451 -1.377 -0.149
0.427 -0.149 -1.366
0.008 -0.028 0.007
-0.011 -0.005 -0.004
0.002 0.002 -0.002

atensor 15 C
-0.268 -0.451 -0.427
-0.451 -1.377 0.149
-0.427 0.149 -1.366
0.008 -0.028 -0.007
-0.011 -0.005 0.004
-0.002 -0.002 -0.002

atensor 16 C
-0.268 0.451 -0.427
0.451 -1.377 -0.149
-0.427 -0.149 -1.366
0.008 0.028 -0.007
0.011 -0.005 -0.004
-0.002 0.002 -0.002

atensor 17 C
-0.020 0.240 0.051
0.240 -0.018 0.023
0.051 0.023 -0.236
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.002

atensor 18 C
-0.020 -0.240 0.051
-0.240 -0.018 -0.023
0.051 -0.023 -0.236
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.002

atensor 19 C
-0.020 -0.240 -0.051
-0.240 -0.018 0.023
-0.051 0.023 -0.236
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 20 C
-0.020 0.240 -0.051
0.240 -0.018 -0.023
-0.051 -0.023 -0.236
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 23 C

0.162 -0.136 0.021
-0.136 0.257 -0.009
0.021 -0.009 0.045
0.000 -0.003 0.000
-0.003 0.002 -0.001
0.000 0.000 -0.001

atensor 24 C
0.162 0.136 0.021
0.136 0.257 0.009
0.021 0.009 0.045
0.000 0.003 0.000
0.003 0.002 0.001
0.000 0.000 -0.001

atensor 25 C
-0.363 0.162 0.313
0.162 -0.820 -0.033
0.313 -0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 0.001
0.002 0.003 -0.002

atensor 26 C
-0.363 -0.162 0.313
-0.162 -0.820 0.033
0.313 0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 -0.001
0.002 -0.003 -0.002

atensor 27 C
-0.363 -0.162 -0.313
-0.162 -0.820 -0.033
-0.313 -0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 0.001
-0.002 0.003 -0.002

atensor 28 C
-0.363 0.162 -0.313
0.162 -0.820 0.033
-0.313 0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 -0.001
-0.002 -0.003 -0.002

atensor 29 C
0.220 0.108 0.044
0.108 0.140 0.051
0.044 0.051 0.058
0.001 0.002 0.001
0.003 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.220 -0.108 0.044
-0.108 0.140 -0.051
0.044 -0.051 0.058
0.001 -0.002 0.001
-0.003 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.220 -0.108 -0.044
-0.108 0.140 0.051
-0.044 0.051 0.058

0.001 -0.002 -0.001
-0.003 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.220 0.108 -0.044
0.108 0.140 -0.051
-0.044 -0.051 0.058
0.001 0.002 -0.001
0.003 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.008 0.091 0.001
0.091 0.034 -0.015
0.001 -0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 34 C
0.008 -0.091 0.001
-0.091 0.034 0.015
0.001 0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 35 C
0.008 -0.091 -0.001
-0.091 0.034 -0.015
-0.001 -0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 36 C
0.008 0.091 -0.001
0.091 0.034 0.015
-0.001 0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 37 C
0.025 0.081 0.032
0.081 0.006 0.014
0.032 0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 38 C
0.025 -0.081 0.032
-0.081 0.005 -0.014
0.032 -0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 39 C
0.025 -0.081 -0.032
-0.081 0.006 0.014
-0.032 0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 40 C
0.025 0.081 -0.032
0.081 0.006 -0.014
-0.032 -0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 41 C
0.041 0.044 -0.008
0.044 0.042 0.021
-0.008 0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.044 -0.008
-0.044 0.042 -0.021
-0.008 -0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.044 0.008
-0.044 0.042 0.021
0.008 0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.044 0.008
0.044 0.042 -0.021
0.008 -0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.583 0.355 0.013
0.355 0.689 0.251
0.013 0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 0.005
0.000 0.002 -0.005

atensor 48 H
-0.583 -0.355 0.013
-0.355 0.689 -0.251
0.013 -0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 49 H
-0.582 -0.355 -0.013
-0.355 0.689 0.251
-0.013 0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 0.005
0.000 0.002 -0.005

atensor 50 H
-0.583 0.355 -0.013

0.355 0.689 -0.251
-0.013 -0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 51 H
-0.103 0.645 -0.164
0.645 0.479 -0.272
-0.164 -0.272 -0.423
-0.002 0.013 -0.003
0.013 0.010 -0.006
-0.002 -0.003 -0.004

atensor 52 H
-0.103 -0.645 -0.164
-0.645 0.479 0.272
-0.164 0.272 -0.423
-0.002 -0.013 -0.003
-0.013 0.010 0.006
-0.002 0.003 -0.004

atensor 53 H
-0.103 -0.645 0.164
-0.645 0.479 -0.272
0.164 -0.272 -0.423
-0.002 -0.013 0.003
-0.013 0.010 -0.006
0.002 -0.003 -0.004

atensor 54 H
-0.103 0.645 0.164
0.645 0.479 0.272
0.164 0.272 -0.423
-0.002 0.013 0.003
0.013 0.010 0.006
0.002 0.003 -0.004

atensor 55 H
0.270 0.445 0.370
0.445 -0.116 0.229
0.371 0.229 -0.203
0.006 0.009 0.007
0.010 -0.002 0.005
0.004 0.003 -0.002

atensor 56 H
0.270 -0.445 0.370
-0.445 -0.116 -0.229
0.371 -0.229 -0.203
0.006 -0.009 0.007
-0.010 -0.002 -0.005
0.004 -0.003 -0.002

atensor 57 H
0.270 -0.445 -0.370
-0.445 -0.116 0.229
-0.371 0.229 -0.203
0.006 -0.009 -0.007
-0.010 -0.002 0.005
-0.004 0.003 -0.002

atensor 58 H
0.270 0.445 -0.370
0.445 -0.116 -0.229
-0.371 -0.229 -0.203
0.006 0.009 -0.007

0.010 -0.002 -0.005
-0.004 -0.003 -0.002

atensor 59 H
0.019 0.235 -0.044
0.235 0.157 -0.062
-0.044 -0.062 -0.139
0.000 0.004 -0.001
0.005 0.003 -0.001
-0.001 -0.001 -0.002

atensor 60 H
0.019 -0.235 -0.044
-0.235 0.157 0.062
-0.044 0.062 -0.139
0.000 -0.004 -0.001
-0.005 0.003 0.001
-0.001 0.001 -0.002

atensor 61 H
0.019 -0.235 0.044
-0.235 0.157 -0.062
0.044 -0.062 -0.139
0.000 -0.004 0.001
-0.005 0.003 -0.001
0.001 -0.001 -0.002

atensor 62 H
0.019 0.235 0.044
0.235 0.157 0.062
0.044 0.062 -0.139
0.000 0.004 0.001
0.005 0.003 0.001
0.001 0.001 -0.002

atensor 63 H
0.616 0.340 0.100
0.340 -0.753 -0.014
0.100 -0.014 -0.727
0.019 0.008 0.001
0.004 -0.013 0.001
0.001 0.001 -0.006

atensor 64 H
0.616 -0.340 0.100
-0.340 -0.753 0.014
0.100 0.014 -0.727
0.019 -0.008 0.001
-0.004 -0.013 -0.001
0.001 -0.001 -0.006

atensor 65 H
0.616 -0.340 -0.100
-0.340 -0.753 -0.014
-0.100 -0.014 -0.727
0.019 -0.008 -0.001
-0.004 -0.013 0.001
-0.001 0.001 -0.006

atensor 66 H
0.616 0.340 -0.100
0.340 -0.753 0.014
-0.100 0.014 -0.727
0.019 0.008 -0.001
0.004 -0.013 -0.001
-0.001 -0.001 -0.006

atensor 67 H
0.118 0.195 0.097
0.195 0.012 0.072
0.097 0.072 -0.095
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.118 -0.195 0.097
-0.195 0.012 -0.072
0.097 -0.072 -0.095
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.118 -0.195 -0.097
-0.195 0.012 0.072
-0.097 0.072 -0.095
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.118 0.195 -0.097
0.195 0.012 -0.072
-0.097 -0.072 -0.095
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.039 0.170 0.012
0.170 0.042 0.017
0.012 0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.039 -0.170 0.012
-0.170 0.042 -0.017
0.012 -0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.039 -0.170 -0.012
-0.170 0.042 0.017
-0.012 0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.039 0.170 -0.012
0.170 0.042 -0.017
-0.012 -0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.368 -17.100 -1.598
-17.100 -306.210 -34.163

-1.598 -34.163 -81.636
261.881 -3.875 -0.979
-3.875 258.313 4.204
-0.979 4.204 222.714

orbtensor 2 C
-220.368 17.100 -1.598
17.100 -306.210 34.163
-1.598 34.163 -81.636
261.881 3.875 -0.979
3.875 258.313 -4.204
-0.979 -4.204 222.714

orbtensor 3 C
-220.368 17.100 1.598
17.100 -306.210 -34.163
1.598 -34.163 -81.636
261.881 3.875 0.979
3.875 258.313 4.204
0.979 4.204 222.714

orbtensor 4 C
-220.368 -17.100 1.598
-17.100 -306.210 34.163
1.598 34.163 -81.636
261.881 -3.875 0.979
-3.875 258.313 -4.204
0.979 -4.204 222.714

orbtensor 5 C
-276.212 -12.908 2.770
-12.908 -296.076 -24.658
2.770 -24.658 -94.207
271.043 2.198 -0.318
2.198 265.976 3.256
-0.318 3.256 228.998

orbtensor 6 C
-276.212 12.908 2.770
12.908 -296.076 24.658
2.770 24.658 -94.207
271.043 -2.198 -0.318
-2.198 265.976 -3.256
-0.318 -3.256 228.998

orbtensor 7 C
-276.212 12.908 -2.770
12.908 -296.076 -24.658
-2.770 -24.658 -94.207
271.043 -2.198 0.318
-2.198 265.976 3.256
0.318 3.256 228.998

orbtensor 8 C
-276.212 -12.909 -2.770
-12.909 -296.076 24.658
-2.770 24.658 -94.207
271.043 2.198 0.318
2.198 265.976 -3.256
0.318 -3.256 228.998

orbtensor 9 C
-251.304 -17.109 8.657
-17.109 -253.695 -10.888
8.657 -10.888 -64.805
262.703 0.702 -0.479
0.702 262.933 0.846

```

-0.479    0.846    217.246

orbtensor 10 C
-251.304    17.109    8.657
17.109 -253.695    10.888
8.657    10.888 -64.805
262.703    -0.702    -0.479
-0.702    262.933    -0.846
-0.479    -0.846    217.246

orbtensor 11 C
-251.304    17.109    -8.657
17.109 -253.695 -10.888
-8.657 -10.888 -64.805
262.703    -0.702    0.479
-0.702    262.933    0.846
0.479    0.846    217.246

orbtensor 12 C
-251.304 -17.109    -8.657
-17.109 -253.695    10.888
-8.657    10.888 -64.805
262.703    0.702    0.479
0.702    262.933    -0.846
0.479    -0.846    217.246

orbtensor 13 C
-291.184    -7.658    29.280
-7.658 -281.792 -13.099
29.280 -13.099 -84.765
266.519    1.965    -1.564
1.965    270.756    0.788
-1.564    0.788    229.036

orbtensor 14 C
-291.184    7.658    29.280
7.658 -281.792    13.099
29.280    13.099 -84.765
266.519    -1.964    -1.564
-1.964    270.756    -0.788
-1.564    -0.788    229.035

orbtensor 15 C
-291.185    7.658    -29.280
7.658 -281.792 -13.099
-29.280 -13.099 -84.765
266.519    -1.965    1.564
-1.965    270.756    0.788
1.564    0.788    229.036

orbtensor 16 C
-291.185    -7.658    -29.280
-7.658 -281.792    13.099
-29.280    13.099 -84.765
266.519    1.964    1.564
1.964    270.756    -0.788
1.564    -0.788    229.035

orbtensor 17 C
-220.617 -107.808 -56.417
-107.808 -218.956    58.673
-56.417    58.673 -210.882
253.914    14.332    9.925
14.332    253.939    -9.934
9.925    -9.934    249.834

orbtensor 18 C

```

```
-220.618  107.808  -56.417
107.808  -218.956  -58.673
-56.417  -58.673  -210.881
253.914  -14.332   9.926
-14.332  253.939   9.934
9.926    9.934   249.834
```

```
orbtensor 19 C
-220.618  107.808   56.417
107.808  -218.956   58.673
56.417   58.673  -210.882
253.914  -14.332   -9.925
-14.332  253.939   -9.934
-9.925   -9.934   249.834
```

```
orbtensor 20 C
-220.618  -107.808   56.417
-107.808  -218.956  -58.673
56.417   -58.673  -210.882
253.914   14.332   -9.926
14.332   253.939   9.934
-9.926    9.934   249.834
```

```
orbtensor 23 C
-199.899   69.717   90.781
69.717  -165.664   49.438
90.781   49.438  -256.373
246.830  -14.814   -6.166
-14.814  250.046  -13.241
-6.166  -13.241   249.107
```

```
orbtensor 24 C
-199.899  -69.717   90.781
-69.717  -165.664  -49.438
90.781  -49.438  -256.373
246.830   14.814   -6.166
14.814  250.046   13.241
-6.166   13.241   249.107
```

```
orbtensor 25 C
-300.040  -14.281   35.998
-14.281  -218.667   12.304
35.998   12.304  -81.318
258.970   -4.022   -3.577
-4.022  261.080    1.056
-3.577   1.056   222.061
```

```
orbtensor 26 C
-300.040   14.281   35.998
14.281  -218.667  -12.304
35.998  -12.304  -81.318
258.970    4.022   -3.577
4.022  261.080   -1.056
-3.577  -1.056   222.061
```

```
orbtensor 27 C
-300.040   14.281  -35.998
14.281  -218.667   12.304
-35.998   12.304  -81.318
258.970    4.022    3.577
4.022  261.080    1.056
3.577   1.056   222.061
```

```
orbtensor 28 C
-300.040  -14.281  -35.998
-14.281  -218.667  -12.304
-35.998  -12.304  -81.318
```


258.970 -4.022 3.577
-4.022 261.080 -1.056
3.577 -1.056 222.061

orbtensor 29 C
-164.840 -67.454 -50.879
-67.454 -194.765 89.528
-50.879 89.528 -257.250
249.711 14.880 13.261
14.880 246.379 -6.422
13.261 -6.422 248.719

orbtensor 30 C
-164.840 67.454 -50.879
67.454 -194.765 -89.528
-50.879 -89.528 -257.250
249.711 -14.880 13.261
-14.880 246.379 6.422
13.261 6.422 248.719

orbtensor 31 C
-164.840 67.454 50.879
67.454 -194.765 89.528
50.879 89.528 -257.250
249.711 -14.880 -13.261
-14.880 246.379 -6.422
-13.261 -6.422 248.719

orbtensor 32 C
-164.840 -67.454 50.879
-67.454 -194.765 -89.528
50.879 -89.528 -257.250
249.711 14.880 -13.261
14.880 246.379 6.422
-13.261 6.422 248.719

orbtensor 33 C
-153.807 -70.075 -47.682
-70.075 -193.288 99.288
-47.682 99.288 -227.224
246.005 15.535 10.652
15.535 243.791 -9.554
10.652 -9.554 245.192

orbtensor 34 C
-153.807 70.075 -47.682
70.075 -193.288 -99.288
-47.682 -99.288 -227.223
246.005 -15.535 10.652
-15.535 243.791 9.554
10.652 9.554 245.192

orbtensor 35 C
-153.807 70.075 47.682
70.075 -193.288 99.288
47.682 99.288 -227.224
246.005 -15.535 -10.652
-15.535 243.791 -9.554
-10.652 -9.554 245.192

orbtensor 36 C
-153.807 -70.075 47.682
-70.075 -193.288 -99.288
47.682 -99.288 -227.223
246.005 15.535 -10.652
15.535 243.791 9.554
-10.652 9.554 245.192

```

gtensor (ppt)
-0.155    0.000    0.000
0.000   -0.154    0.000
0.000    0.000   -0.239
39.011    0.000    0.000
0.000   41.659    0.000
0.000    0.000   21.064

```

```

zfstensor (cm-1)
1.964053    0.000010    0.000321
0.000010    1.840828   -0.000123
0.000321   -0.000123   -73.369452

```

```

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4307	44.89800	223.02581	-6.07963	216.94617	261.84417
2	C	-0.4307	44.89800	223.02581	-6.07948	216.94633	261.84433
3	C	-0.4307	44.89800	223.02581	-6.07958	216.94622	261.84422
4	C	-0.4307	44.89800	223.02581	-6.07942	216.94639	261.84439
5	C	-1.2237	33.17400	633.69020	25.62263	659.31283	692.48683
6	C	-1.2237	33.17400	633.69020	25.62287	659.31307	692.48707
7	C	-1.2237	33.17400	633.69020	25.62232	659.31252	692.48652
8	C	-1.2237	33.17400	633.69020	25.62259	659.31279	692.48679
9	C	0.4570	57.69267	-236.66283	0.89764	-235.76520	-178.07253
10	C	0.4570	57.69267	-236.66283	0.89762	-235.76521	-178.07255
11	C	0.4570	57.69267	-236.66283	0.89718	-235.76565	-178.07299
12	C	0.4570	57.69267	-236.66283	0.89721	-235.76562	-178.07296
13	C	-1.0033	36.19000	519.58799	27.39279	546.98078	583.17078
14	C	-1.0033	36.18967	519.58799	27.39285	546.98084	583.17051
15	C	-1.0033	36.18967	519.58799	27.39222	546.98020	583.16987
16	C	-1.0033	36.18933	519.58799	27.39231	546.98029	583.16963
17	C	-0.0907	35.74400	46.95280	10.99977	57.95257	93.69657
18	C	-0.0907	35.74400	46.95280	10.99977	57.95258	93.69658
19	C	-0.0907	35.74367	46.95280	10.99970	57.95250	93.69616
20	C	-0.0907	35.74367	46.95280	10.99971	57.95252	93.69618
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1550	41.34900	-80.26858	8.27300	-71.99557	-30.64657
24	C	0.1550	41.34900	-80.26858	8.27300	-71.99557	-30.64657
25	C	-0.6483	47.36200	335.74705	7.14159	342.88864	390.25064
26	C	-0.6483	47.36200	335.74705	7.14157	342.88862	390.25062
27	C	-0.6483	47.36200	335.74705	7.14117	342.88823	390.25023
28	C	-0.6483	47.36200	335.74705	7.14116	342.88822	390.25022
29	C	0.1393	42.65133	-72.15541	6.15910	-65.99631	-23.34498
30	C	0.1393	42.65133	-72.15541	6.15912	-65.99629	-23.34496
31	C	0.1393	42.65133	-72.15541	6.15903	-65.99637	-23.34504
32	C	0.1393	42.65133	-72.15541	6.15906	-65.99634	-23.34501
33	C	-0.0050	53.55633	2.58931	3.95303	6.54234	60.09867
34	C	-0.0050	53.55667	2.58931	3.95302	6.54233	60.09900
35	C	-0.0050	53.55633	2.58931	3.95303	6.54234	60.09867
36	C	-0.0050	53.55667	2.58931	3.95302	6.54233	60.09900
A Average		-1.1135	34.68183	576.63909	26.50757	603.14666	637.82850
B Average		-0.5395	46.13000	279.38643	0.53092	279.91735	326.04735
M Average		0.4570	57.69267	-236.66283	0.89741	-235.76542	-178.07276

```

=====
FeL5-saddled-LS-STO-PBE0-No-ZFS
Temperature: 303

```

Spin: 1.5

atensor 1 C

-0.630 0.186 -0.043
0.186 -0.290 0.319
-0.043 0.319 -0.349
-0.033 -0.005 -0.001
0.009 0.011 0.002
-0.003 0.000 -0.001

atensor 2 C

-0.630 -0.186 -0.043
-0.186 -0.290 -0.319
-0.043 -0.319 -0.349
-0.033 0.005 -0.001
-0.009 0.011 -0.002
-0.003 0.000 -0.001

atensor 3 C

-0.630 -0.186 0.043
-0.186 -0.290 0.319
0.043 0.319 -0.349
-0.033 0.005 0.001
-0.009 0.011 0.002
0.003 0.000 -0.001

atensor 4 C

-0.630 0.186 0.043
0.186 -0.290 -0.319
0.043 -0.319 -0.349
-0.033 -0.005 0.001
0.009 0.011 -0.002
0.003 0.000 -0.001

atensor 5 C

-1.576 0.460 0.220
0.460 -0.512 0.514
0.220 0.514 -1.568
-0.016 0.016 0.007
0.035 0.002 0.006
0.004 0.001 -0.001

atensor 6 C

-1.576 -0.460 0.220
-0.460 -0.512 -0.514
0.220 -0.514 -1.568
-0.016 -0.016 0.007
-0.035 0.002 -0.006
0.004 -0.001 -0.001

atensor 7 C

-1.576 -0.460 -0.220
-0.460 -0.512 0.514
-0.220 0.514 -1.568
-0.016 -0.016 -0.007
-0.035 0.002 0.006
-0.004 0.001 -0.001

atensor 8 C

-1.576 0.460 -0.220
0.460 -0.512 -0.514
-0.220 -0.514 -1.568
-0.016 0.016 -0.007
0.035 0.002 -0.006
-0.004 -0.001 -0.001

atensor 9 C

0.464 0.671 0.328
0.671 0.455 0.011
0.328 0.011 0.448
0.004 0.008 0.002
0.004 0.003 0.002
0.003 0.002 -0.003

atensor 10 C
0.464 -0.671 0.328
-0.671 0.455 -0.011
0.328 -0.011 0.448
0.004 -0.008 0.002
-0.004 0.003 -0.002
0.003 -0.002 -0.003

atensor 11 C
0.464 -0.671 -0.328
-0.671 0.455 0.011
-0.328 0.011 0.448
0.004 -0.008 -0.002
-0.004 0.003 0.002
-0.003 0.002 -0.003

atensor 12 C
0.464 0.671 -0.328
0.671 0.455 -0.011
-0.328 -0.011 0.448
0.004 0.008 -0.002
0.004 0.003 -0.002
-0.003 -0.002 -0.003

atensor 13 C
-0.268 0.451 0.427
0.451 -1.377 0.149
0.427 0.149 -1.366
0.008 0.028 0.007
0.011 -0.005 0.004
0.002 -0.002 -0.002

atensor 14 C
-0.268 -0.451 0.427
-0.451 -1.377 -0.149
0.427 -0.149 -1.366
0.008 -0.028 0.007
-0.011 -0.005 -0.004
0.002 0.002 -0.002

atensor 15 C
-0.268 -0.451 -0.427
-0.451 -1.377 0.149
-0.427 0.149 -1.366
0.008 -0.028 -0.007
-0.011 -0.005 0.004
-0.002 -0.002 -0.002

atensor 16 C
-0.268 0.451 -0.427
0.451 -1.377 -0.149
-0.427 -0.149 -1.366
0.008 0.028 -0.007
0.011 -0.005 -0.004
-0.002 0.002 -0.002

atensor 17 C
-0.020 0.240 0.051
0.240 -0.018 0.023
0.051 0.023 -0.236

0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.002

atensor 18 C
-0.020 -0.240 0.051
-0.240 -0.018 -0.023
0.051 -0.023 -0.236
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.002

atensor 19 C
-0.020 -0.240 -0.051
-0.240 -0.018 0.023
-0.051 0.023 -0.236
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 20 C
-0.020 0.240 -0.051
0.240 -0.018 -0.023
-0.051 -0.023 -0.236
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 23 C
0.162 -0.136 0.021
-0.136 0.257 -0.009
0.021 -0.009 0.045
0.000 -0.003 0.000
-0.003 0.002 -0.001
0.000 0.000 -0.001

atensor 24 C
0.162 0.136 0.021
0.136 0.257 0.009
0.021 0.009 0.045
0.000 0.003 0.000
0.003 0.002 0.001
0.000 0.000 -0.001

atensor 25 C
-0.363 0.162 0.313
0.162 -0.820 -0.033
0.313 -0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 0.001
0.002 0.003 -0.002

atensor 26 C
-0.363 -0.162 0.313
-0.162 -0.820 0.033
0.313 0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 -0.001
0.002 -0.003 -0.002

atensor 27 C
-0.363 -0.162 -0.313
-0.162 -0.820 -0.033
-0.313 -0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 0.001
-0.002 0.003 -0.002

atensor 28 C
-0.363 0.162 -0.313
0.162 -0.820 0.033
-0.313 0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 -0.001
-0.002 -0.003 -0.002

atensor 29 C
0.220 0.108 0.044
0.108 0.140 0.051
0.044 0.051 0.058
0.001 0.002 0.001
0.003 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.220 -0.108 0.044
-0.108 0.140 -0.051
0.044 -0.051 0.058
0.001 -0.002 0.001
-0.003 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.220 -0.108 -0.044
-0.108 0.140 0.051
-0.044 0.051 0.058
0.001 -0.002 -0.001
-0.003 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.220 0.108 -0.044
0.108 0.140 -0.051
-0.044 -0.051 0.058
0.001 0.002 -0.001
0.003 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.008 0.091 0.001
0.091 0.034 -0.015
0.001 -0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 34 C
0.008 -0.091 0.001
-0.091 0.034 0.015
0.001 0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 35 C
0.008 -0.091 -0.001
-0.091 0.034 -0.015
-0.001 -0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 36 C
0.008 0.091 -0.001

0.091 0.034 0.015
-0.001 0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 37 C
0.025 0.081 0.032
0.081 0.006 0.014
0.032 0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 38 C
0.025 -0.081 0.032
-0.081 0.005 -0.014
0.032 -0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 39 C
0.025 -0.081 -0.032
-0.081 0.006 0.014
-0.032 0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 40 C
0.025 0.081 -0.032
0.081 0.006 -0.014
-0.032 -0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 41 C
0.041 0.044 -0.008
0.044 0.042 0.021
-0.008 0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.044 -0.008
-0.044 0.042 -0.021
-0.008 -0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.044 0.008
-0.044 0.042 0.021
0.008 0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.044 0.008
0.044 0.042 -0.021
0.008 -0.021 -0.024
0.000 0.001 0.000

0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.583 0.355 0.013
0.355 0.689 0.251
0.013 0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 0.005
0.000 0.002 -0.005

atensor 48 H
-0.583 -0.355 0.013
-0.355 0.689 -0.251
0.013 -0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 49 H
-0.582 -0.355 -0.013
-0.355 0.689 0.251
-0.013 0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 0.005
0.000 0.002 -0.005

atensor 50 H
-0.583 0.355 -0.013
0.355 0.689 -0.251
-0.013 -0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 51 H
-0.103 0.645 -0.164
0.645 0.479 -0.272
-0.164 -0.272 -0.423
-0.002 0.013 -0.003
0.013 0.010 -0.006
-0.002 -0.003 -0.004

atensor 52 H
-0.103 -0.645 -0.164
-0.645 0.479 0.272
-0.164 0.272 -0.423
-0.002 -0.013 -0.003
-0.013 0.010 0.006
-0.002 0.003 -0.004

atensor 53 H
-0.103 -0.645 0.164
-0.645 0.479 -0.272
0.164 -0.272 -0.423
-0.002 -0.013 0.003
-0.013 0.010 -0.006
0.002 -0.003 -0.004

atensor 54 H
-0.103 0.645 0.164
0.645 0.479 0.272
0.164 0.272 -0.423
-0.002 0.013 0.003
0.013 0.010 0.006
0.002 0.003 -0.004

atensor 55 H
0.270 0.445 0.370
0.445 -0.116 0.229
0.371 0.229 -0.203
0.006 0.009 0.007
0.010 -0.002 0.005
0.004 0.003 -0.002

atensor 56 H
0.270 -0.445 0.370
-0.445 -0.116 -0.229
0.371 -0.229 -0.203
0.006 -0.009 0.007
-0.010 -0.002 -0.005
0.004 -0.003 -0.002

atensor 57 H
0.270 -0.445 -0.370
-0.445 -0.116 0.229
-0.371 0.229 -0.203
0.006 -0.009 -0.007
-0.010 -0.002 0.005
-0.004 0.003 -0.002

atensor 58 H
0.270 0.445 -0.370
0.445 -0.116 -0.229
-0.371 -0.229 -0.203
0.006 0.009 -0.007
0.010 -0.002 -0.005
-0.004 -0.003 -0.002

atensor 59 H
0.019 0.235 -0.044
0.235 0.157 -0.062
-0.044 -0.062 -0.139
0.000 0.004 -0.001
0.005 0.003 -0.001
-0.001 -0.001 -0.002

atensor 60 H
0.019 -0.235 -0.044
-0.235 0.157 0.062
-0.044 0.062 -0.139
0.000 -0.004 -0.001
-0.005 0.003 0.001
-0.001 0.001 -0.002

atensor 61 H
0.019 -0.235 0.044
-0.235 0.157 -0.062
0.044 -0.062 -0.139
0.000 -0.004 0.001
-0.005 0.003 -0.001
0.001 -0.001 -0.002

atensor 62 H
0.019 0.235 0.044
0.235 0.157 0.062
0.044 0.062 -0.139
0.000 0.004 0.001
0.005 0.003 0.001
0.001 0.001 -0.002

atensor 63 H
0.616 0.340 0.100
0.340 -0.753 -0.014

0.100 -0.014 -0.727
0.019 0.008 0.001
0.004 -0.013 0.001
0.001 0.001 -0.006

atensor 64 H
0.616 -0.340 0.100
-0.340 -0.753 0.014
0.100 0.014 -0.727
0.019 -0.008 0.001
-0.004 -0.013 -0.001
0.001 -0.001 -0.006

atensor 65 H
0.616 -0.340 -0.100
-0.340 -0.753 -0.014
-0.100 -0.014 -0.727
0.019 -0.008 -0.001
-0.004 -0.013 0.001
-0.001 0.001 -0.006

atensor 66 H
0.616 0.340 -0.100
0.340 -0.753 0.014
-0.100 0.014 -0.727
0.019 0.008 -0.001
0.004 -0.013 -0.001
-0.001 -0.001 -0.006

atensor 67 H
0.118 0.195 0.097
0.195 0.012 0.072
0.097 0.072 -0.095
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.118 -0.195 0.097
-0.195 0.012 -0.072
0.097 -0.072 -0.095
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.118 -0.195 -0.097
-0.195 0.012 0.072
-0.097 0.072 -0.095
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.118 0.195 -0.097
0.195 0.012 -0.072
-0.097 -0.072 -0.095
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.039 0.170 0.012
0.170 0.042 0.017
0.012 0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000

0.000 0.000 -0.001

atensor 72 H
0.039 -0.170 0.012
-0.170 0.042 -0.017
0.012 -0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.039 -0.170 -0.012
-0.170 0.042 0.017
-0.012 0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.039 0.170 -0.012
0.170 0.042 -0.017
-0.012 -0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.368 -17.100 -1.598
-17.100 -306.210 -34.163
-1.598 -34.163 -81.636
261.881 -3.875 -0.979
-3.875 258.313 4.204
-0.979 4.204 222.714

orbtensor 2 C
-220.368 17.100 -1.598
17.100 -306.210 34.163
-1.598 34.163 -81.636
261.881 3.875 -0.979
3.875 258.313 -4.204
-0.979 -4.204 222.714

orbtensor 3 C
-220.368 17.100 1.598
17.100 -306.210 -34.163
1.598 -34.163 -81.636
261.881 3.875 0.979
3.875 258.313 4.204
0.979 4.204 222.714

orbtensor 4 C
-220.368 -17.100 1.598
-17.100 -306.210 34.163
1.598 34.163 -81.636
261.881 -3.875 0.979
-3.875 258.313 -4.204
0.979 -4.204 222.714

orbtensor 5 C
-276.212 -12.908 2.770
-12.908 -296.076 -24.658
2.770 -24.658 -94.207
271.043 2.198 -0.318
2.198 265.976 3.256
-0.318 3.256 228.998

orbtensor 6 C

```
-276.212  12.908  2.770
12.908 -296.076  24.658
2.770  24.658 -94.207
271.043  -2.198  -0.318
-2.198  265.976  -3.256
-0.318  -3.256  228.998
```

```
orbtensor 7 C
-276.212  12.908  -2.770
12.908 -296.076  -24.658
-2.770 -24.658  -94.207
271.043  -2.198  0.318
-2.198  265.976  3.256
0.318  3.256  228.998
```

```
orbtensor 8 C
-276.212  -12.909  -2.770
-12.909 -296.076  24.658
-2.770  24.658  -94.207
271.043  2.198  0.318
2.198  265.976  -3.256
0.318  -3.256  228.998
```

```
orbtensor 9 C
-251.304  -17.109  8.657
-17.109 -253.695  -10.888
8.657 -10.888  -64.805
262.703  0.702  -0.479
0.702  262.933  0.846
-0.479  0.846  217.246
```

```
orbtensor 10 C
-251.304  17.109  8.657
17.109 -253.695  10.888
8.657  10.888  -64.805
262.703  -0.702  -0.479
-0.702  262.933  -0.846
-0.479  -0.846  217.246
```

```
orbtensor 11 C
-251.304  17.109  -8.657
17.109 -253.695  -10.888
-8.657 -10.888  -64.805
262.703  -0.702  0.479
-0.702  262.933  0.846
0.479  0.846  217.246
```

```
orbtensor 12 C
-251.304  -17.109  -8.657
-17.109 -253.695  10.888
-8.657  10.888  -64.805
262.703  0.702  0.479
0.702  262.933  -0.846
0.479  -0.846  217.246
```

```
orbtensor 13 C
-291.184  -7.658  29.280
-7.658 -281.792  -13.099
29.280 -13.099  -84.765
266.519  1.965  -1.564
1.965  270.756  0.788
-1.564  0.788  229.036
```

```
orbtensor 14 C
-291.184  7.658  29.280
7.658 -281.792  13.099
29.280  13.099  -84.765
```

266.519 -1.964 -1.564
-1.964 270.756 -0.788
-1.564 -0.788 229.035

orbtensor 15 C
-291.185 7.658 -29.280
7.658 -281.792 -13.099
-29.280 -13.099 -84.765
266.519 -1.965 1.564
-1.965 270.756 0.788
1.564 0.788 229.036

orbtensor 16 C
-291.185 -7.658 -29.280
-7.658 -281.792 13.099
-29.280 13.099 -84.765
266.519 1.964 1.564
1.964 270.756 -0.788
1.564 -0.788 229.035

orbtensor 17 C
-220.617 -107.808 -56.417
-107.808 -218.956 58.673
-56.417 58.673 -210.882
253.914 14.332 9.925
14.332 253.939 -9.934
9.925 -9.934 249.834

orbtensor 18 C
-220.618 107.808 -56.417
107.808 -218.956 -58.673
-56.417 -58.673 -210.881
253.914 -14.332 9.926
-14.332 253.939 9.934
9.926 9.934 249.834

orbtensor 19 C
-220.618 107.808 56.417
107.808 -218.956 58.673
56.417 58.673 -210.882
253.914 -14.332 -9.925
-14.332 253.939 -9.934
-9.925 -9.934 249.834

orbtensor 20 C
-220.618 -107.808 56.417
-107.808 -218.956 -58.673
56.417 -58.673 -210.882
253.914 14.332 -9.926
14.332 253.939 9.934
-9.926 9.934 249.834

orbtensor 23 C
-199.899 69.717 90.781
69.717 -165.664 49.438
90.781 49.438 -256.373
246.830 -14.814 -6.166
-14.814 250.046 -13.241
-6.166 -13.241 249.107

orbtensor 24 C
-199.899 -69.717 90.781
-69.717 -165.664 -49.438
90.781 -49.438 -256.373
246.830 14.814 -6.166
14.814 250.046 13.241
-6.166 13.241 249.107

orbtensor 25 C
-300.040 -14.281 35.998
-14.281 -218.667 12.304
35.998 12.304 -81.318
258.970 -4.022 -3.577
-4.022 261.080 1.056
-3.577 1.056 222.061

orbtensor 26 C
-300.040 14.281 35.998
14.281 -218.667 -12.304
35.998 -12.304 -81.318
258.970 4.022 -3.577
4.022 261.080 -1.056
-3.577 -1.056 222.061

orbtensor 27 C
-300.040 14.281 -35.998
14.281 -218.667 12.304
-35.998 12.304 -81.318
258.970 4.022 3.577
4.022 261.080 1.056
3.577 1.056 222.061

orbtensor 28 C
-300.040 -14.281 -35.998
-14.281 -218.667 -12.304
-35.998 -12.304 -81.318
258.970 -4.022 3.577
-4.022 261.080 -1.056
3.577 -1.056 222.061

orbtensor 29 C
-164.840 -67.454 -50.879
-67.454 -194.765 89.528
-50.879 89.528 -257.250
249.711 14.880 13.261
14.880 246.379 -6.422
13.261 -6.422 248.719

orbtensor 30 C
-164.840 67.454 -50.879
67.454 -194.765 -89.528
-50.879 -89.528 -257.250
249.711 -14.880 13.261
-14.880 246.379 6.422
13.261 6.422 248.719

orbtensor 31 C
-164.840 67.454 50.879
67.454 -194.765 89.528
50.879 89.528 -257.250
249.711 -14.880 -13.261
-14.880 246.379 -6.422
-13.261 -6.422 248.719

orbtensor 32 C
-164.840 -67.454 50.879
-67.454 -194.765 -89.528
50.879 -89.528 -257.250
249.711 14.880 -13.261
14.880 246.379 6.422
-13.261 6.422 248.719

orbtensor 33 C
-153.807 -70.075 -47.682

```

-70.075  -193.288   99.288
-47.682   99.288  -227.224
246.005   15.535   10.652
15.535   243.791  -9.554
10.652   -9.554   245.192

```

```

orbtensor 34 C
-153.807   70.075  -47.682
70.075  -193.288  -99.288
-47.682  -99.288  -227.223
246.005  -15.535   10.652
-15.535  243.791   9.554
10.652   9.554   245.192

```

```

orbtensor 35 C
-153.807   70.075   47.682
70.075  -193.288   99.288
47.682   99.288  -227.224
246.005  -15.535  -10.652
-15.535  243.791  -9.554
-10.652  -9.554   245.192

```

```

orbtensor 36 C
-153.807  -70.075   47.682
-70.075  -193.288  -99.288
47.682  -99.288  -227.223
246.005   15.535  -10.652
15.535   243.791   9.554
-10.652   9.554   245.192

```

```

gtensor (ppt)
-0.155   0.000   0.000
0.000  -0.154   0.000
0.000   0.000  -0.239
39.011   0.000   0.000
0.000   41.659   0.000
0.000   0.000   21.064

```

```

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4307	44.89800	226.91203	0.09081	227.00284	271.90084
2	C	-0.4307	44.89800	226.91203	0.09081	227.00284	271.90084
3	C	-0.4307	44.89800	226.91203	0.09081	227.00284	271.90084
4	C	-0.4307	44.89800	226.91203	0.09081	227.00284	271.90084
5	C	-1.2237	33.17400	644.73226	-0.70019	644.03207	677.20607
6	C	-1.2237	33.17400	644.73226	-0.70019	644.03207	677.20607
7	C	-1.2237	33.17400	644.73226	-0.70019	644.03207	677.20607
8	C	-1.2237	33.17400	644.73226	-0.70019	644.03207	677.20607
9	C	0.4570	57.69267	-240.78669	-0.01889	-240.80558	-183.11291
10	C	0.4570	57.69267	-240.78669	-0.01889	-240.80558	-183.11291
11	C	0.4570	57.69267	-240.78669	-0.01889	-240.80558	-183.11291
12	C	0.4570	57.69267	-240.78669	-0.01889	-240.80558	-183.11291
13	C	-1.0033	36.19000	528.64181	-0.48066	528.16116	564.35116
14	C	-1.0033	36.18967	528.64181	-0.48066	528.16116	564.35082
15	C	-1.0033	36.18967	528.64181	-0.48066	528.16116	564.35082
16	C	-1.0033	36.18933	528.64181	-0.48066	528.16116	564.35049
17	C	-0.0907	35.74400	47.77095	-0.24622	47.52474	83.26874
18	C	-0.0907	35.74400	47.77095	-0.24622	47.52474	83.26874
19	C	-0.0907	35.74367	47.77095	-0.24622	47.52474	83.26841
20	C	-0.0907	35.74367	47.77095	-0.24622	47.52474	83.26841

21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1550	41.34900	-81.66726	-0.19641	-81.86366	-40.51466
24	C	0.1550	41.34900	-81.66726	-0.19641	-81.86366	-40.51466
25	C	-0.6483	47.36200	341.59745	-0.10139	341.49606	388.85806
26	C	-0.6483	47.36200	341.59745	-0.10139	341.49606	388.85806
27	C	-0.6483	47.36200	341.59745	-0.10139	341.49606	388.85806
28	C	-0.6483	47.36200	341.59745	-0.10139	341.49606	388.85806
29	C	0.1393	42.65133	-73.41272	-0.12821	-73.54093	-30.88959
30	C	0.1393	42.65133	-73.41272	-0.12821	-73.54093	-30.88959
31	C	0.1393	42.65133	-73.41272	-0.12821	-73.54093	-30.88959
32	C	0.1393	42.65133	-73.41272	-0.12821	-73.54093	-30.88959
33	C	-0.0050	53.55633	2.63443	-0.09157	2.54285	56.09919
34	C	-0.0050	53.55667	2.63443	-0.09157	2.54285	56.09952
35	C	-0.0050	53.55633	2.63443	-0.09157	2.54285	56.09919
36	C	-0.0050	53.55667	2.63443	-0.09157	2.54285	56.09952
A Average		-1.1135	34.68183	586.68704	-0.59042	586.09661	620.77845
B Average		-0.5395	46.13000	284.25474	-0.00529	284.24945	330.37945
M Average		0.4570	57.69267	-240.78669	-0.01889	-240.80558	-183.11291

=====

FeL5-saddled-LS-STO-PBE0-No-G

Temperature: 303

Spin: 1.5

atensor 1 C

-0.630 0.186 -0.043
0.186 -0.290 0.319
-0.043 0.319 -0.349
-0.033 -0.005 -0.001
0.009 0.011 0.002
-0.003 0.000 -0.001

atensor 2 C

-0.630 -0.186 -0.043
-0.186 -0.290 -0.319
-0.043 -0.319 -0.349
-0.033 0.005 -0.001
-0.009 0.011 -0.002
-0.003 0.000 -0.001

atensor 3 C

-0.630 -0.186 0.043
-0.186 -0.290 0.319
0.043 0.319 -0.349
-0.033 0.005 0.001
-0.009 0.011 0.002
0.003 0.000 -0.001

atensor 4 C

-0.630 0.186 0.043
0.186 -0.290 -0.319
0.043 -0.319 -0.349
-0.033 -0.005 0.001
0.009 0.011 -0.002
0.003 0.000 -0.001

atensor 5 C

-1.576 0.460 0.220
0.460 -0.512 0.514
0.220 0.514 -1.568
-0.016 0.016 0.007
0.035 0.002 0.006
0.004 0.001 -0.001

atensor 6 C

-1.576 -0.460 0.220
-0.460 -0.512 -0.514
0.220 -0.514 -1.568
-0.016 -0.016 0.007
-0.035 0.002 -0.006
0.004 -0.001 -0.001

atensor 7 C
-1.576 -0.460 -0.220
-0.460 -0.512 0.514
-0.220 0.514 -1.568
-0.016 -0.016 -0.007
-0.035 0.002 0.006
-0.004 0.001 -0.001

atensor 8 C
-1.576 0.460 -0.220
0.460 -0.512 -0.514
-0.220 -0.514 -1.568
-0.016 0.016 -0.007
0.035 0.002 -0.006
-0.004 -0.001 -0.001

atensor 9 C
0.464 0.671 0.328
0.671 0.455 0.011
0.328 0.011 0.448
0.004 0.008 0.002
0.004 0.003 0.002
0.003 0.002 -0.003

atensor 10 C
0.464 -0.671 0.328
-0.671 0.455 -0.011
0.328 -0.011 0.448
0.004 -0.008 0.002
-0.004 0.003 -0.002
0.003 -0.002 -0.003

atensor 11 C
0.464 -0.671 -0.328
-0.671 0.455 0.011
-0.328 0.011 0.448
0.004 -0.008 -0.002
-0.004 0.003 0.002
-0.003 0.002 -0.003

atensor 12 C
0.464 0.671 -0.328
0.671 0.455 -0.011
-0.328 -0.011 0.448
0.004 0.008 -0.002
0.004 0.003 -0.002
-0.003 -0.002 -0.003

atensor 13 C
-0.268 0.451 0.427
0.451 -1.377 0.149
0.427 0.149 -1.366
0.008 0.028 0.007
0.011 -0.005 0.004
0.002 -0.002 -0.002

atensor 14 C
-0.268 -0.451 0.427
-0.451 -1.377 -0.149
0.427 -0.149 -1.366

0.008 -0.028 0.007
-0.011 -0.005 -0.004
0.002 0.002 -0.002

atensor 15 C
-0.268 -0.451 -0.427
-0.451 -1.377 0.149
-0.427 0.149 -1.366
0.008 -0.028 -0.007
-0.011 -0.005 0.004
-0.002 -0.002 -0.002

atensor 16 C
-0.268 0.451 -0.427
0.451 -1.377 -0.149
-0.427 -0.149 -1.366
0.008 0.028 -0.007
0.011 -0.005 -0.004
-0.002 0.002 -0.002

atensor 17 C
-0.020 0.240 0.051
0.240 -0.018 0.023
0.051 0.023 -0.236
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.002

atensor 18 C
-0.020 -0.240 0.051
-0.240 -0.018 -0.023
0.051 -0.023 -0.236
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.002

atensor 19 C
-0.020 -0.240 -0.051
-0.240 -0.018 0.023
-0.051 0.023 -0.236
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 20 C
-0.020 0.240 -0.051
0.240 -0.018 -0.023
-0.051 -0.023 -0.236
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.002

atensor 23 C
0.162 -0.136 0.021
-0.136 0.257 -0.009
0.021 -0.009 0.045
0.000 -0.003 0.000
-0.003 0.002 -0.001
0.000 0.000 -0.001

atensor 24 C
0.162 0.136 0.021
0.136 0.257 0.009
0.021 0.009 0.045
0.000 0.003 0.000
0.003 0.002 0.001
0.000 0.000 -0.001

atensor 25 C
-0.363 0.162 0.313
0.162 -0.820 -0.033
0.313 -0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 0.001
0.002 0.003 -0.002

atensor 26 C
-0.363 -0.162 0.313
-0.162 -0.820 0.033
0.313 0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 -0.001
0.002 -0.003 -0.002

atensor 27 C
-0.363 -0.162 -0.313
-0.162 -0.820 -0.033
-0.313 -0.033 -0.741
0.010 -0.005 0.000
0.001 -0.029 0.001
-0.002 0.003 -0.002

atensor 28 C
-0.363 0.162 -0.313
0.162 -0.820 0.033
-0.313 0.033 -0.741
0.010 0.005 0.000
-0.001 -0.029 -0.001
-0.002 -0.003 -0.002

atensor 29 C
0.220 0.108 0.044
0.108 0.140 0.051
0.044 0.051 0.058
0.001 0.002 0.001
0.003 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.220 -0.108 0.044
-0.108 0.140 -0.051
0.044 -0.051 0.058
0.001 -0.002 0.001
-0.003 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.220 -0.108 -0.044
-0.108 0.140 0.051
-0.044 0.051 0.058
0.001 -0.002 -0.001
-0.003 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.220 0.108 -0.044
0.108 0.140 -0.051
-0.044 -0.051 0.058
0.001 0.002 -0.001
0.003 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.008 0.091 0.001

0.091 0.034 -0.015
0.001 -0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 34 C
0.008 -0.091 0.001
-0.091 0.034 0.015
0.001 0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 35 C
0.008 -0.091 -0.001
-0.091 0.034 -0.015
-0.001 -0.015 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 36 C
0.008 0.091 -0.001
0.091 0.034 0.015
-0.001 0.015 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 37 C
0.025 0.081 0.032
0.081 0.006 0.014
0.032 0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 38 C
0.025 -0.081 0.032
-0.081 0.005 -0.014
0.032 -0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 39 C
0.025 -0.081 -0.032
-0.081 0.006 0.014
-0.032 0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 40 C
0.025 0.081 -0.032
0.081 0.006 -0.014
-0.032 -0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 41 C
0.041 0.044 -0.008
0.044 0.042 0.021
-0.008 0.021 -0.024
0.000 0.001 0.000

0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.044 -0.008
-0.044 0.042 -0.021
-0.008 -0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.044 0.008
-0.044 0.042 0.021
0.008 0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.044 0.008
0.044 0.042 -0.021
0.008 -0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.583 0.355 0.013
0.355 0.689 0.251
0.013 0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 0.005
0.000 0.002 -0.005

atensor 48 H
-0.583 -0.355 0.013
-0.355 0.689 -0.251
0.013 -0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 49 H
-0.582 -0.355 -0.013
-0.355 0.689 0.251
-0.013 0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 0.005
0.000 0.002 -0.005

atensor 50 H
-0.583 0.355 -0.013
0.355 0.689 -0.251
-0.013 -0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 51 H
-0.103 0.645 -0.164
0.645 0.479 -0.272
-0.164 -0.272 -0.423
-0.002 0.013 -0.003
0.013 0.010 -0.006
-0.002 -0.003 -0.004

atensor 52 H
-0.103 -0.645 -0.164
-0.645 0.479 0.272
-0.164 0.272 -0.423
-0.002 -0.013 -0.003
-0.013 0.010 0.006
-0.002 0.003 -0.004

atensor 53 H
-0.103 -0.645 0.164
-0.645 0.479 -0.272
0.164 -0.272 -0.423
-0.002 -0.013 0.003
-0.013 0.010 -0.006
0.002 -0.003 -0.004

atensor 54 H
-0.103 0.645 0.164
0.645 0.479 0.272
0.164 0.272 -0.423
-0.002 0.013 0.003
0.013 0.010 0.006
0.002 0.003 -0.004

atensor 55 H
0.270 0.445 0.370
0.445 -0.116 0.229
0.371 0.229 -0.203
0.006 0.009 0.007
0.010 -0.002 0.005
0.004 0.003 -0.002

atensor 56 H
0.270 -0.445 0.370
-0.445 -0.116 -0.229
0.371 -0.229 -0.203
0.006 -0.009 0.007
-0.010 -0.002 -0.005
0.004 -0.003 -0.002

atensor 57 H
0.270 -0.445 -0.370
-0.445 -0.116 0.229
-0.371 0.229 -0.203
0.006 -0.009 -0.007
-0.010 -0.002 0.005
-0.004 0.003 -0.002

atensor 58 H
0.270 0.445 -0.370
0.445 -0.116 -0.229
-0.371 -0.229 -0.203
0.006 0.009 -0.007
0.010 -0.002 -0.005
-0.004 -0.003 -0.002

atensor 59 H
0.019 0.235 -0.044
0.235 0.157 -0.062
-0.044 -0.062 -0.139
0.000 0.004 -0.001
0.005 0.003 -0.001
-0.001 -0.001 -0.002

atensor 60 H
0.019 -0.235 -0.044
-0.235 0.157 0.062

-0.044 0.062 -0.139
0.000 -0.004 -0.001
-0.005 0.003 0.001
-0.001 0.001 -0.002

atensor 61 H
0.019 -0.235 0.044
-0.235 0.157 -0.062
0.044 -0.062 -0.139
0.000 -0.004 0.001
-0.005 0.003 -0.001
0.001 -0.001 -0.002

atensor 62 H
0.019 0.235 0.044
0.235 0.157 0.062
0.044 0.062 -0.139
0.000 0.004 0.001
0.005 0.003 0.001
0.001 0.001 -0.002

atensor 63 H
0.616 0.340 0.100
0.340 -0.753 -0.014
0.100 -0.014 -0.727
0.019 0.008 0.001
0.004 -0.013 0.001
0.001 0.001 -0.006

atensor 64 H
0.616 -0.340 0.100
-0.340 -0.753 0.014
0.100 0.014 -0.727
0.019 -0.008 0.001
-0.004 -0.013 -0.001
0.001 -0.001 -0.006

atensor 65 H
0.616 -0.340 -0.100
-0.340 -0.753 -0.014
-0.100 -0.014 -0.727
0.019 -0.008 -0.001
-0.004 -0.013 0.001
-0.001 0.001 -0.006

atensor 66 H
0.616 0.340 -0.100
0.340 -0.753 0.014
-0.100 0.014 -0.727
0.019 0.008 -0.001
0.004 -0.013 -0.001
-0.001 -0.001 -0.006

atensor 67 H
0.118 0.195 0.097
0.195 0.012 0.072
0.097 0.072 -0.095
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.118 -0.195 0.097
-0.195 0.012 -0.072
0.097 -0.072 -0.095
0.002 -0.004 0.002
-0.004 0.000 -0.002

0.001 -0.001 -0.001

atensor 69 H
0.118 -0.195 -0.097
-0.195 0.012 0.072
-0.097 0.072 -0.095
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.118 0.195 -0.097
0.195 0.012 -0.072
-0.097 -0.072 -0.095
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.039 0.170 0.012
0.170 0.042 0.017
0.012 0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.039 -0.170 0.012
-0.170 0.042 -0.017
0.012 -0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.039 -0.170 -0.012
-0.170 0.042 0.017
-0.012 0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.039 0.170 -0.012
0.170 0.042 -0.017
-0.012 -0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.368 -17.100 -1.598
-17.100 -306.210 -34.163
-1.598 -34.163 -81.636
261.881 -3.875 -0.979
-3.875 258.313 4.204
-0.979 4.204 222.714

orbtensor 2 C
-220.368 17.100 -1.598
17.100 -306.210 34.163
-1.598 34.163 -81.636
261.881 3.875 -0.979
3.875 258.313 -4.204
-0.979 -4.204 222.714

orbtensor 3 C


```
-220.368  17.100  1.598
17.100 -306.210 -34.163
1.598 -34.163 -81.636
261.881  3.875  0.979
3.875 258.313  4.204
0.979  4.204 222.714
```

```
orbtensor 4 C
-220.368 -17.100  1.598
-17.100 -306.210  34.163
1.598  34.163 -81.636
261.881 -3.875  0.979
-3.875 258.313 -4.204
0.979 -4.204 222.714
```

```
orbtensor 5 C
-276.212 -12.908  2.770
-12.908 -296.076 -24.658
2.770 -24.658 -94.207
271.043  2.198 -0.318
2.198 265.976  3.256
-0.318  3.256 228.998
```

```
orbtensor 6 C
-276.212  12.908  2.770
12.908 -296.076  24.658
2.770  24.658 -94.207
271.043 -2.198 -0.318
-2.198 265.976 -3.256
-0.318 -3.256 228.998
```

```
orbtensor 7 C
-276.212  12.908 -2.770
12.908 -296.076 -24.658
-2.770 -24.658 -94.207
271.043 -2.198  0.318
-2.198 265.976  3.256
0.318  3.256 228.998
```

```
orbtensor 8 C
-276.212 -12.909 -2.770
-12.909 -296.076  24.658
-2.770  24.658 -94.207
271.043  2.198  0.318
2.198 265.976 -3.256
0.318 -3.256 228.998
```

```
orbtensor 9 C
-251.304 -17.109  8.657
-17.109 -253.695 -10.888
8.657 -10.888 -64.805
262.703  0.702 -0.479
0.702 262.933  0.846
-0.479  0.846 217.246
```

```
orbtensor 10 C
-251.304  17.109  8.657
17.109 -253.695  10.888
8.657  10.888 -64.805
262.703 -0.702 -0.479
-0.702 262.933 -0.846
-0.479 -0.846 217.246
```

```
orbtensor 11 C
-251.304  17.109 -8.657
17.109 -253.695 -10.888
-8.657 -10.888 -64.805
```

262.703 -0.702 0.479
-0.702 262.933 0.846
0.479 0.846 217.246

orbtensor 12 C
-251.304 -17.109 -8.657
-17.109 -253.695 10.888
-8.657 10.888 -64.805
262.703 0.702 0.479
0.702 262.933 -0.846
0.479 -0.846 217.246

orbtensor 13 C
-291.184 -7.658 29.280
-7.658 -281.792 -13.099
29.280 -13.099 -84.765
266.519 1.965 -1.564
1.965 270.756 0.788
-1.564 0.788 229.036

orbtensor 14 C
-291.184 7.658 29.280
7.658 -281.792 13.099
29.280 13.099 -84.765
266.519 -1.964 -1.564
-1.964 270.756 -0.788
-1.564 -0.788 229.035

orbtensor 15 C
-291.185 7.658 -29.280
7.658 -281.792 -13.099
-29.280 -13.099 -84.765
266.519 -1.965 1.564
-1.965 270.756 0.788
1.564 0.788 229.036

orbtensor 16 C
-291.185 -7.658 -29.280
-7.658 -281.792 13.099
-29.280 13.099 -84.765
266.519 1.964 1.564
1.964 270.756 -0.788
1.564 -0.788 229.035

orbtensor 17 C
-220.617 -107.808 -56.417
-107.808 -218.956 58.673
-56.417 58.673 -210.882
253.914 14.332 9.925
14.332 253.939 -9.934
9.925 -9.934 249.834

orbtensor 18 C
-220.618 107.808 -56.417
107.808 -218.956 -58.673
-56.417 -58.673 -210.881
253.914 -14.332 9.926
-14.332 253.939 9.934
9.926 9.934 249.834

orbtensor 19 C
-220.618 107.808 56.417
107.808 -218.956 58.673
56.417 58.673 -210.882
253.914 -14.332 -9.925
-14.332 253.939 -9.934
-9.925 -9.934 249.834

orbtensor 20 C
-220.618 -107.808 56.417
-107.808 -218.956 -58.673
56.417 -58.673 -210.882
253.914 14.332 -9.926
14.332 253.939 9.934
-9.926 9.934 249.834

orbtensor 23 C
-199.899 69.717 90.781
69.717 -165.664 49.438
90.781 49.438 -256.373
246.830 -14.814 -6.166
-14.814 250.046 -13.241
-6.166 -13.241 249.107

orbtensor 24 C
-199.899 -69.717 90.781
-69.717 -165.664 -49.438
90.781 -49.438 -256.373
246.830 14.814 -6.166
14.814 250.046 13.241
-6.166 13.241 249.107

orbtensor 25 C
-300.040 -14.281 35.998
-14.281 -218.667 12.304
35.998 12.304 -81.318
258.970 -4.022 -3.577
-4.022 261.080 1.056
-3.577 1.056 222.061

orbtensor 26 C
-300.040 14.281 35.998
14.281 -218.667 -12.304
35.998 -12.304 -81.318
258.970 4.022 -3.577
4.022 261.080 -1.056
-3.577 -1.056 222.061

orbtensor 27 C
-300.040 14.281 -35.998
14.281 -218.667 12.304
-35.998 12.304 -81.318
258.970 4.022 3.577
4.022 261.080 1.056
3.577 1.056 222.061

orbtensor 28 C
-300.040 -14.281 -35.998
-14.281 -218.667 -12.304
-35.998 -12.304 -81.318
258.970 -4.022 3.577
-4.022 261.080 -1.056
3.577 -1.056 222.061

orbtensor 29 C
-164.840 -67.454 -50.879
-67.454 -194.765 89.528
-50.879 89.528 -257.250
249.711 14.880 13.261
14.880 246.379 -6.422
13.261 -6.422 248.719

orbtensor 30 C
-164.840 67.454 -50.879

```
67.454 -194.765 -89.528
-50.879 -89.528 -257.250
249.711 -14.880 13.261
-14.880 246.379 6.422
13.261 6.422 248.719
```

```
orbtensor 31 C
-164.840 67.454 50.879
67.454 -194.765 89.528
50.879 89.528 -257.250
249.711 -14.880 -13.261
-14.880 246.379 -6.422
-13.261 -6.422 248.719
```

```
orbtensor 32 C
-164.840 -67.454 50.879
-67.454 -194.765 -89.528
50.879 -89.528 -257.250
249.711 14.880 -13.261
14.880 246.379 6.422
-13.261 6.422 248.719
```

```
orbtensor 33 C
-153.807 -70.075 -47.682
-70.075 -193.288 99.288
-47.682 99.288 -227.224
246.005 15.535 10.652
15.535 243.791 -9.554
10.652 -9.554 245.192
```

```
orbtensor 34 C
-153.807 70.075 -47.682
70.075 -193.288 -99.288
-47.682 -99.288 -227.223
246.005 -15.535 10.652
-15.535 243.791 9.554
10.652 9.554 245.192
```

```
orbtensor 35 C
-153.807 70.075 47.682
70.075 -193.288 99.288
47.682 99.288 -227.224
246.005 -15.535 -10.652
-15.535 243.791 -9.554
-10.652 -9.554 245.192
```

```
orbtensor 36 C
-153.807 -70.075 47.682
-70.075 -193.288 -99.288
47.682 -99.288 -227.223
246.005 15.535 -10.652
15.535 243.791 9.554
-10.652 9.554 245.192
```

```
gtensor (ppt)
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
```

```
averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12
```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4307	44.89800	223.15307	-0.00000	223.15307	268.05107
2	C	-0.4307	44.89800	223.15307	-0.00000	223.15307	268.05107
3	C	-0.4307	44.89800	223.15307	-0.00000	223.15307	268.05107
4	C	-0.4307	44.89800	223.15307	-0.00000	223.15307	268.05107
5	C	-1.2237	33.17400	634.05178	-0.00000	634.05178	667.22578
6	C	-1.2237	33.17400	634.05178	-0.00000	634.05178	667.22578
7	C	-1.2237	33.17400	634.05178	-0.00000	634.05178	667.22578
8	C	-1.2237	33.17400	634.05178	-0.00000	634.05178	667.22578
9	C	0.4570	57.69267	-236.79787	-0.00000	-236.79787	-179.10521
10	C	0.4570	57.69267	-236.79787	-0.00000	-236.79787	-179.10521
11	C	0.4570	57.69267	-236.79787	-0.00000	-236.79787	-179.10521
12	C	0.4570	57.69267	-236.79787	-0.00000	-236.79787	-179.10521
13	C	-1.0033	36.19000	519.88446	0.00000	519.88446	556.07446
14	C	-1.0033	36.18967	519.88446	0.00000	519.88446	556.07413
15	C	-1.0033	36.18967	519.88446	0.00000	519.88446	556.07413
16	C	-1.0033	36.18933	519.88446	0.00000	519.88446	556.07380
17	C	-0.0907	35.74400	46.97959	0.00000	46.97959	82.72359
18	C	-0.0907	35.74400	46.97959	0.00000	46.97959	82.72359
19	C	-0.0907	35.74367	46.97959	0.00000	46.97959	82.72326
20	C	-0.0907	35.74367	46.97959	0.00000	46.97959	82.72326
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1550	41.34900	-80.31438	0.00000	-80.31438	-38.96538
24	C	0.1550	41.34900	-80.31438	0.00000	-80.31438	-38.96538
25	C	-0.6483	47.36200	335.93863	0.00000	335.93863	383.30063
26	C	-0.6483	47.36200	335.93863	0.00000	335.93863	383.30063
27	C	-0.6483	47.36200	335.93863	0.00000	335.93863	383.30063
28	C	-0.6483	47.36200	335.93863	0.00000	335.93863	383.30063
29	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
30	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
31	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
32	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
33	C	-0.0050	53.55633	2.59079	0.00000	2.59079	56.14712
34	C	-0.0050	53.55667	2.59079	0.00000	2.59079	56.14745
35	C	-0.0050	53.55633	2.59079	0.00000	2.59079	56.14712
36	C	-0.0050	53.55667	2.59079	0.00000	2.59079	56.14745
A Average		-1.1135	34.68183	576.96812	-0.00000	576.96812	611.64996
B Average		-0.5395	46.13000	279.54585	-0.00000	279.54585	325.67585
M Average		0.4570	57.69267	-236.79787	-0.00000	-236.79787	-179.10521

=====
 FeL5-saddled-LS-STO-PBE0-No-PSOSO
 Temperature: 303
 Spin: 1.5

atensor 1 C
 -0.630 0.186 -0.043
 0.186 -0.290 0.319
 -0.043 0.319 -0.349
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

atensor 2 C
 -0.630 -0.186 -0.043
 -0.186 -0.290 -0.319
 -0.043 -0.319 -0.349
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

atensor 3 C

-0.630 -0.186 0.043
-0.186 -0.290 0.319
0.043 0.319 -0.349
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 C
-0.630 0.186 0.043
0.186 -0.290 -0.319
0.043 -0.319 -0.349
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
-1.576 0.460 0.220
0.460 -0.512 0.514
0.220 0.514 -1.568
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 C
-1.576 -0.460 0.220
-0.460 -0.512 -0.514
0.220 -0.514 -1.568
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
-1.576 -0.460 -0.220
-0.460 -0.512 0.514
-0.220 0.514 -1.568
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 C
-1.576 0.460 -0.220
0.460 -0.512 -0.514
-0.220 -0.514 -1.568
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.464 0.671 0.328
0.671 0.455 0.011
0.328 0.011 0.448
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 C
0.464 -0.671 0.328
-0.671 0.455 -0.011
0.328 -0.011 0.448
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.464 -0.671 -0.328
-0.671 0.455 0.011
-0.328 0.011 0.448

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 C

0.464 0.671 -0.328
0.671 0.455 -0.011
-0.328 -0.011 0.448
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C

-0.268 0.451 0.427
0.451 -1.377 0.149
0.427 0.149 -1.366
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 C

-0.268 -0.451 0.427
-0.451 -1.377 -0.149
0.427 -0.149 -1.366
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C

-0.268 -0.451 -0.427
-0.451 -1.377 0.149
-0.427 0.149 -1.366
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 C

-0.268 0.451 -0.427
0.451 -1.377 -0.149
-0.427 -0.149 -1.366
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C

-0.020 0.240 0.051
0.240 -0.018 0.023
0.051 0.023 -0.236
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 C

-0.020 -0.240 0.051
-0.240 -0.018 -0.023
0.051 -0.023 -0.236
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C

-0.020 -0.240 -0.051
-0.240 -0.018 0.023
-0.051 0.023 -0.236
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.020 0.240 -0.051
0.240 -0.018 -0.023
-0.051 -0.023 -0.236
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.162 -0.136 0.021
-0.136 0.257 -0.009
0.021 -0.009 0.045
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 C
0.162 0.136 0.021
0.136 0.257 0.009
0.021 0.009 0.045
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 C
-0.363 0.162 0.313
0.162 -0.820 -0.033
0.313 -0.033 -0.741
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 C
-0.363 -0.162 0.313
-0.162 -0.820 0.033
0.313 0.033 -0.741
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 C
-0.363 -0.162 -0.313
-0.162 -0.820 -0.033
-0.313 -0.033 -0.741
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 C
-0.363 0.162 -0.313
0.162 -0.820 0.033
-0.313 0.033 -0.741
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 29 C
0.220 0.108 0.044
0.108 0.140 0.051
0.044 0.051 0.058
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.220 -0.108 0.044

-0.108 0.140 -0.051
0.044 -0.051 0.058
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.220 -0.108 -0.044
-0.108 0.140 0.051
-0.044 0.051 0.058
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.220 0.108 -0.044
0.108 0.140 -0.051
-0.044 -0.051 0.058
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.008 0.091 0.001
0.091 0.034 -0.015
0.001 -0.015 -0.057
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.008 -0.091 0.001
-0.091 0.034 0.015
0.001 0.015 -0.057
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.008 -0.091 -0.001
-0.091 0.034 -0.015
-0.001 -0.015 -0.057
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.008 0.091 -0.001
0.091 0.034 0.015
-0.001 0.015 -0.057
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.025 0.081 0.032
0.081 0.006 0.014
0.032 0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 38 C
0.025 -0.081 0.032
-0.081 0.005 -0.014
0.032 -0.014 -0.046
0.001 -0.001 0.000

-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 39 C
0.025 -0.081 -0.032
-0.081 0.006 0.014
-0.032 0.014 -0.046
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 40 C
0.025 0.081 -0.032
0.081 0.006 -0.014
-0.032 -0.014 -0.046
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 41 C
0.041 0.044 -0.008
0.044 0.042 0.021
-0.008 0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.044 -0.008
-0.044 0.042 -0.021
-0.008 -0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.044 0.008
-0.044 0.042 0.021
0.008 0.021 -0.024
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.044 0.008
0.044 0.042 -0.021
0.008 -0.021 -0.024
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.583 0.355 0.013
0.355 0.689 0.251
0.013 0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 0.005
0.000 0.002 -0.005

atensor 48 H
-0.583 -0.355 0.013
-0.355 0.689 -0.251
0.013 -0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 49 H
-0.582 -0.355 -0.013
-0.355 0.689 0.251
-0.013 0.251 -0.528
-0.013 -0.002 0.000
-0.008 0.019 0.005
0.000 0.002 -0.005

atensor 50 H
-0.583 0.355 -0.013
0.355 0.689 -0.251
-0.013 -0.251 -0.528
-0.013 0.002 0.000
0.008 0.019 -0.005
0.000 -0.002 -0.005

atensor 51 H
-0.103 0.645 -0.164
0.645 0.479 -0.272
-0.164 -0.272 -0.423
-0.002 0.013 -0.003
0.013 0.010 -0.006
-0.002 -0.003 -0.004

atensor 52 H
-0.103 -0.645 -0.164
-0.645 0.479 0.272
-0.164 0.272 -0.423
-0.002 -0.013 -0.003
-0.013 0.010 0.006
-0.002 0.003 -0.004

atensor 53 H
-0.103 -0.645 0.164
-0.645 0.479 -0.272
0.164 -0.272 -0.423
-0.002 -0.013 0.003
-0.013 0.010 -0.006
0.002 -0.003 -0.004

atensor 54 H
-0.103 0.645 0.164
0.645 0.479 0.272
0.164 0.272 -0.423
-0.002 0.013 0.003
0.013 0.010 0.006
0.002 0.003 -0.004

atensor 55 H
0.270 0.445 0.370
0.445 -0.116 0.229
0.371 0.229 -0.203
0.006 0.009 0.007
0.010 -0.002 0.005
0.004 0.003 -0.002

atensor 56 H
0.270 -0.445 0.370
-0.445 -0.116 -0.229
0.371 -0.229 -0.203
0.006 -0.009 0.007
-0.010 -0.002 -0.005
0.004 -0.003 -0.002

atensor 57 H
0.270 -0.445 -0.370
-0.445 -0.116 0.229

-0.371 0.229 -0.203
0.006 -0.009 -0.007
-0.010 -0.002 0.005
-0.004 0.003 -0.002

atensor 58 H
0.270 0.445 -0.370
0.445 -0.116 -0.229
-0.371 -0.229 -0.203
0.006 0.009 -0.007
0.010 -0.002 -0.005
-0.004 -0.003 -0.002

atensor 59 H
0.019 0.235 -0.044
0.235 0.157 -0.062
-0.044 -0.062 -0.139
0.000 0.004 -0.001
0.005 0.003 -0.001
-0.001 -0.001 -0.002

atensor 60 H
0.019 -0.235 -0.044
-0.235 0.157 0.062
-0.044 0.062 -0.139
0.000 -0.004 -0.001
-0.005 0.003 0.001
-0.001 0.001 -0.002

atensor 61 H
0.019 -0.235 0.044
-0.235 0.157 -0.062
0.044 -0.062 -0.139
0.000 -0.004 0.001
-0.005 0.003 -0.001
0.001 -0.001 -0.002

atensor 62 H
0.019 0.235 0.044
0.235 0.157 0.062
0.044 0.062 -0.139
0.000 0.004 0.001
0.005 0.003 0.001
0.001 0.001 -0.002

atensor 63 H
0.616 0.340 0.100
0.340 -0.753 -0.014
0.100 -0.014 -0.727
0.019 0.008 0.001
0.004 -0.013 0.001
0.001 0.001 -0.006

atensor 64 H
0.616 -0.340 0.100
-0.340 -0.753 0.014
0.100 0.014 -0.727
0.019 -0.008 0.001
-0.004 -0.013 -0.001
0.001 -0.001 -0.006

atensor 65 H
0.616 -0.340 -0.100
-0.340 -0.753 -0.014
-0.100 -0.014 -0.727
0.019 -0.008 -0.001
-0.004 -0.013 0.001

-0.001 0.001 -0.006

atensor 66 H
0.616 0.340 -0.100
0.340 -0.753 0.014
-0.100 0.014 -0.727
0.019 0.008 -0.001
0.004 -0.013 -0.001
-0.001 -0.001 -0.006

atensor 67 H
0.118 0.195 0.097
0.195 0.012 0.072
0.097 0.072 -0.095
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.118 -0.195 0.097
-0.195 0.012 -0.072
0.097 -0.072 -0.095
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.118 -0.195 -0.097
-0.195 0.012 0.072
-0.097 0.072 -0.095
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.118 0.195 -0.097
0.195 0.012 -0.072
-0.097 -0.072 -0.095
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.039 0.170 0.012
0.170 0.042 0.017
0.012 0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.039 -0.170 0.012
-0.170 0.042 -0.017
0.012 -0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.039 -0.170 -0.012
-0.170 0.042 0.017
-0.012 0.017 -0.131
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H

0.039 0.170 -0.012
0.170 0.042 -0.017
-0.012 -0.017 -0.131
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.368 -17.100 -1.598
-17.100 -306.210 -34.163
-1.598 -34.163 -81.636
261.881 -3.875 -0.979
-3.875 258.313 4.204
-0.979 4.204 222.714

orbtensor 2 C
-220.368 17.100 -1.598
17.100 -306.210 34.163
-1.598 34.163 -81.636
261.881 3.875 -0.979
3.875 258.313 -4.204
-0.979 -4.204 222.714

orbtensor 3 C
-220.368 17.100 1.598
17.100 -306.210 -34.163
1.598 -34.163 -81.636
261.881 3.875 0.979
3.875 258.313 4.204
0.979 4.204 222.714

orbtensor 4 C
-220.368 -17.100 1.598
-17.100 -306.210 34.163
1.598 34.163 -81.636
261.881 -3.875 0.979
-3.875 258.313 -4.204
0.979 -4.204 222.714

orbtensor 5 C
-276.212 -12.908 2.770
-12.908 -296.076 -24.658
2.770 -24.658 -94.207
271.043 2.198 -0.318
2.198 265.976 3.256
-0.318 3.256 228.998

orbtensor 6 C
-276.212 12.908 2.770
12.908 -296.076 24.658
2.770 24.658 -94.207
271.043 -2.198 -0.318
-2.198 265.976 -3.256
-0.318 -3.256 228.998

orbtensor 7 C
-276.212 12.908 -2.770
12.908 -296.076 -24.658
-2.770 -24.658 -94.207
271.043 -2.198 0.318
-2.198 265.976 3.256
0.318 3.256 228.998

orbtensor 8 C
-276.212 -12.909 -2.770
-12.909 -296.076 24.658
-2.770 24.658 -94.207

271.043 2.198 0.318
2.198 265.976 -3.256
0.318 -3.256 228.998

orbtensor 9 C
-251.304 -17.109 8.657
-17.109 -253.695 -10.888
8.657 -10.888 -64.805
262.703 0.702 -0.479
0.702 262.933 0.846
-0.479 0.846 217.246

orbtensor 10 C
-251.304 17.109 8.657
17.109 -253.695 10.888
8.657 10.888 -64.805
262.703 -0.702 -0.479
-0.702 262.933 -0.846
-0.479 -0.846 217.246

orbtensor 11 C
-251.304 17.109 -8.657
17.109 -253.695 -10.888
-8.657 -10.888 -64.805
262.703 -0.702 0.479
-0.702 262.933 0.846
0.479 0.846 217.246

orbtensor 12 C
-251.304 -17.109 -8.657
-17.109 -253.695 10.888
-8.657 10.888 -64.805
262.703 0.702 0.479
0.702 262.933 -0.846
0.479 -0.846 217.246

orbtensor 13 C
-291.184 -7.658 29.280
-7.658 -281.792 -13.099
29.280 -13.099 -84.765
266.519 1.965 -1.564
1.965 270.756 0.788
-1.564 0.788 229.036

orbtensor 14 C
-291.184 7.658 29.280
7.658 -281.792 13.099
29.280 13.099 -84.765
266.519 -1.964 -1.564
-1.964 270.756 -0.788
-1.564 -0.788 229.035

orbtensor 15 C
-291.185 7.658 -29.280
7.658 -281.792 -13.099
-29.280 -13.099 -84.765
266.519 -1.965 1.564
-1.965 270.756 0.788
1.564 0.788 229.036

orbtensor 16 C
-291.185 -7.658 -29.280
-7.658 -281.792 13.099
-29.280 13.099 -84.765
266.519 1.964 1.564
1.964 270.756 -0.788
1.564 -0.788 229.035

orbtensor 17 C
-220.617 -107.808 -56.417
-107.808 -218.956 58.673
-56.417 58.673 -210.882
253.914 14.332 9.925
14.332 253.939 -9.934
9.925 -9.934 249.834

orbtensor 18 C
-220.618 107.808 -56.417
107.808 -218.956 -58.673
-56.417 -58.673 -210.881
253.914 -14.332 9.926
-14.332 253.939 9.934
9.926 9.934 249.834

orbtensor 19 C
-220.618 107.808 56.417
107.808 -218.956 58.673
56.417 58.673 -210.882
253.914 -14.332 -9.925
-14.332 253.939 -9.934
-9.925 -9.934 249.834

orbtensor 20 C
-220.618 -107.808 56.417
-107.808 -218.956 -58.673
56.417 -58.673 -210.882
253.914 14.332 -9.926
14.332 253.939 9.934
-9.926 9.934 249.834

orbtensor 23 C
-199.899 69.717 90.781
69.717 -165.664 49.438
90.781 49.438 -256.373
246.830 -14.814 -6.166
-14.814 250.046 -13.241
-6.166 -13.241 249.107

orbtensor 24 C
-199.899 -69.717 90.781
-69.717 -165.664 -49.438
90.781 -49.438 -256.373
246.830 14.814 -6.166
14.814 250.046 13.241
-6.166 13.241 249.107

orbtensor 25 C
-300.040 -14.281 35.998
-14.281 -218.667 12.304
35.998 12.304 -81.318
258.970 -4.022 -3.577
-4.022 261.080 1.056
-3.577 1.056 222.061

orbtensor 26 C
-300.040 14.281 35.998
14.281 -218.667 -12.304
35.998 -12.304 -81.318
258.970 4.022 -3.577
4.022 261.080 -1.056
-3.577 -1.056 222.061

orbtensor 27 C
-300.040 14.281 -35.998

14.281	-218.667	12.304
-35.998	12.304	-81.318
258.970	4.022	3.577
4.022	261.080	1.056
3.577	1.056	222.061

orbtensor 28 C

-300.040	-14.281	-35.998
-14.281	-218.667	-12.304
-35.998	-12.304	-81.318
258.970	-4.022	3.577
-4.022	261.080	-1.056
3.577	-1.056	222.061

orbtensor 29 C

-164.840	-67.454	-50.879
-67.454	-194.765	89.528
-50.879	89.528	-257.250
249.711	14.880	13.261
14.880	246.379	-6.422
13.261	-6.422	248.719

orbtensor 30 C

-164.840	67.454	-50.879
67.454	-194.765	-89.528
-50.879	-89.528	-257.250
249.711	-14.880	13.261
-14.880	246.379	6.422
13.261	6.422	248.719

orbtensor 31 C

-164.840	67.454	50.879
67.454	-194.765	89.528
50.879	89.528	-257.250
249.711	-14.880	-13.261
-14.880	246.379	-6.422
-13.261	-6.422	248.719

orbtensor 32 C

-164.840	-67.454	50.879
-67.454	-194.765	-89.528
50.879	-89.528	-257.250
249.711	14.880	-13.261
14.880	246.379	6.422
-13.261	6.422	248.719

orbtensor 33 C

-153.807	-70.075	-47.682
-70.075	-193.288	99.288
-47.682	99.288	-227.224
246.005	15.535	10.652
15.535	243.791	-9.554
10.652	-9.554	245.192

orbtensor 34 C

-153.807	70.075	-47.682
70.075	-193.288	-99.288
-47.682	-99.288	-227.223
246.005	-15.535	10.652
-15.535	243.791	9.554
10.652	9.554	245.192

orbtensor 35 C

-153.807	70.075	47.682
70.075	-193.288	99.288
47.682	99.288	-227.224
246.005	-15.535	-10.652

-15.535 243.791 -9.554
 -10.652 -9.554 245.192

orbtensor 36 C
 -153.807 -70.075 47.682
 -70.075 -193.288 -99.288
 47.682 -99.288 -227.223
 246.005 15.535 -10.652
 15.535 243.791 9.554
 -10.652 9.554 245.192

gtensor (ppt)
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

averaging
 A Average:5,6,7,8,13,14,15,16
 B Average:1,2,3,4,25,26,27,28
 M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4230	44.89800	219.18053	-0.00000	219.18053	264.07853
2	C	-0.4230	44.89800	219.18053	-0.00000	219.18053	264.07853
3	C	-0.4230	44.89800	219.18053	-0.00000	219.18053	264.07853
4	C	-0.4230	44.89800	219.18053	-0.00000	219.18053	264.07853
5	C	-1.2187	33.17400	631.46100	-0.00000	631.46100	664.63500
6	C	-1.2187	33.17400	631.46100	-0.00000	631.46100	664.63500
7	C	-1.2187	33.17400	631.46100	-0.00000	631.46100	664.63500
8	C	-1.2187	33.17400	631.46100	-0.00000	631.46100	664.63500
9	C	0.4557	57.69267	-236.10700	-0.00000	-236.10700	-178.41433
10	C	0.4557	57.69267	-236.10700	-0.00000	-236.10700	-178.41433
11	C	0.4557	57.69267	-236.10700	-0.00000	-236.10700	-178.41433
12	C	0.4557	57.69267	-236.10700	-0.00000	-236.10700	-178.41433
13	C	-1.0037	36.19000	520.05718	0.00000	520.05718	556.24718
14	C	-1.0037	36.18967	520.05718	0.00000	520.05718	556.24685
15	C	-1.0037	36.18967	520.05718	0.00000	520.05718	556.24685
16	C	-1.0037	36.18933	520.05718	0.00000	520.05718	556.24652
17	C	-0.0913	35.74400	47.32503	0.00000	47.32503	83.06903
18	C	-0.0913	35.74400	47.32503	0.00000	47.32503	83.06903
19	C	-0.0913	35.74367	47.32503	0.00000	47.32503	83.06870
20	C	-0.0913	35.74367	47.32503	0.00000	47.32503	83.06870
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1547	41.34900	-80.14166	0.00000	-80.14166	-38.79266
24	C	0.1547	41.34900	-80.14166	0.00000	-80.14166	-38.79266
25	C	-0.6413	47.36200	332.31153	0.00000	332.31153	379.67353
26	C	-0.6413	47.36200	332.31153	0.00000	332.31153	379.67353
27	C	-0.6413	47.36200	332.31153	0.00000	332.31153	379.67353
28	C	-0.6413	47.36200	332.31153	0.00000	332.31153	379.67353
29	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
30	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
31	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
32	C	0.1393	42.65133	-72.19658	0.00000	-72.19658	-29.54525
33	C	-0.0050	53.55633	2.59079	0.00000	2.59079	56.14712
34	C	-0.0050	53.55667	2.59079	0.00000	2.59079	56.14745
35	C	-0.0050	53.55633	2.59079	0.00000	2.59079	56.14712
36	C	-0.0050	53.55667	2.59079	0.00000	2.59079	56.14745
A Average		-1.1112	34.68183	575.75909	-0.00000	575.75909	610.44092
B Average		-0.5322	46.13000	275.74603	0.00000	275.74603	321.87603

M Average 0.4557 57.69267 -236.10700 -0.00000 -236.10700 -178.41433

=====

FeL5-saddled-LS-STO-PBE0-No-ZORA

Temperature: 303

Spin: 1.5

atensor 1 C

-0.620 0.190 -0.046
0.190 -0.292 0.333
-0.046 0.333 -0.341
-0.033 -0.004 -0.001
0.009 0.011 0.002
-0.003 0.000 -0.001

atensor 2 C

-0.620 -0.190 -0.046
-0.190 -0.292 -0.333
-0.046 -0.333 -0.341
-0.033 0.004 -0.001
-0.009 0.011 -0.002
-0.003 0.000 -0.001

atensor 3 C

-0.620 -0.190 0.046
-0.190 -0.292 0.333
0.046 0.333 -0.341
-0.033 0.004 0.001
-0.009 0.011 0.002
0.003 0.000 -0.001

atensor 4 C

-0.620 0.190 0.046
0.190 -0.292 -0.333
0.046 -0.333 -0.341
-0.033 -0.004 0.001
0.009 0.011 -0.002
0.003 0.000 -0.001

atensor 5 C

-1.565 0.461 0.226
0.461 -0.512 0.524
0.226 0.524 -1.550
-0.015 0.016 0.008
0.035 0.003 0.006
0.005 0.001 -0.001

atensor 6 C

-1.565 -0.461 0.226
-0.461 -0.512 -0.524
0.226 -0.524 -1.550
-0.015 -0.016 0.008
-0.035 0.003 -0.006
0.005 -0.001 -0.001

atensor 7 C

-1.565 -0.461 -0.226
-0.461 -0.512 0.524
-0.226 0.524 -1.550
-0.015 -0.016 -0.008
-0.035 0.003 0.006
-0.005 0.001 -0.001

atensor 8 C

-1.565 0.461 -0.226
0.461 -0.512 -0.524
-0.226 -0.524 -1.550

-0.015 0.016 -0.008
0.035 0.003 -0.006
-0.005 -0.001 -0.001

atensor 9 C
0.473 0.673 0.354
0.673 0.460 -0.015
0.354 -0.015 0.375
0.004 0.009 0.002
0.004 0.003 0.002
0.003 0.002 -0.004

atensor 10 C
0.473 -0.673 0.354
-0.673 0.460 0.015
0.354 0.015 0.375
0.004 -0.009 0.002
-0.004 0.003 -0.002
0.003 -0.002 -0.004

atensor 11 C
0.473 -0.673 -0.354
-0.673 0.460 -0.015
-0.354 -0.015 0.375
0.004 -0.009 -0.002
-0.004 0.003 0.002
-0.003 0.002 -0.004

atensor 12 C
0.473 0.673 -0.354
0.673 0.460 0.015
-0.354 0.015 0.375
0.004 0.009 -0.002
0.004 0.003 -0.002
-0.003 -0.002 -0.004

atensor 13 C
-0.274 0.443 0.422
0.443 -1.378 0.141
0.422 0.141 -1.325
0.009 0.028 0.007
0.011 -0.005 0.004
0.002 -0.002 -0.003

atensor 14 C
-0.275 -0.443 0.422
-0.443 -1.378 -0.141
0.422 -0.141 -1.325
0.009 -0.028 0.007
-0.011 -0.005 -0.004
0.002 0.002 -0.003

atensor 15 C
-0.275 -0.443 -0.422
-0.443 -1.378 0.141
-0.422 0.141 -1.325
0.009 -0.028 -0.007
-0.011 -0.005 0.004
-0.002 -0.002 -0.003

atensor 16 C
-0.275 0.443 -0.422
0.443 -1.378 -0.141
-0.422 -0.141 -1.325
0.009 0.028 -0.007
0.011 -0.005 -0.004
-0.002 0.002 -0.003

```
atensor 17 C
-0.003 0.239 0.050
0.239 -0.001 0.025
0.050 0.025 -0.220
0.002 0.005 0.001
0.005 0.002 0.000
0.001 0.000 -0.002

atensor 18 C
-0.003 -0.239 0.050
-0.239 -0.001 -0.025
0.050 -0.025 -0.220
0.002 -0.005 0.001
-0.005 0.002 0.000
0.001 0.000 -0.002

atensor 19 C
-0.003 -0.239 -0.050
-0.239 -0.001 0.025
-0.050 0.025 -0.220
0.002 -0.005 -0.001
-0.005 0.002 0.000
-0.001 0.000 -0.002

atensor 20 C
-0.003 0.239 -0.050
0.239 -0.001 -0.025
-0.050 -0.025 -0.220
0.002 0.005 -0.001
0.005 0.002 0.000
-0.001 0.000 -0.002

atensor 23 C
0.147 -0.139 0.020
-0.139 0.239 -0.009
0.020 -0.009 0.031
0.000 -0.003 0.000
-0.003 0.002 -0.001
0.000 0.000 -0.001

atensor 24 C
0.147 0.138 0.020
0.138 0.239 0.009
0.020 0.009 0.031
0.000 0.003 0.000
0.003 0.002 0.001
0.000 0.000 -0.001

atensor 25 C
-0.399 0.165 0.319
0.165 -0.841 -0.034
0.319 -0.034 -0.754
0.010 0.005 0.000
-0.001 -0.029 0.001
0.002 0.003 -0.002

atensor 26 C
-0.399 -0.165 0.319
-0.165 -0.841 0.034
0.319 0.034 -0.754
0.010 -0.005 0.000
0.001 -0.029 -0.001
0.002 -0.003 -0.002

atensor 27 C
-0.399 -0.165 -0.319
```

-0.165 -0.841 -0.034
-0.319 -0.034 -0.754
0.010 -0.005 0.000
0.001 -0.029 0.001
-0.002 0.003 -0.002

atensor 28 C
-0.399 0.165 -0.319
0.165 -0.841 0.034
-0.319 0.034 -0.754
0.010 0.005 0.000
-0.001 -0.029 -0.001
-0.002 -0.003 -0.002

atensor 29 C
0.199 0.109 0.045
0.109 0.123 0.051
0.045 0.051 0.042
0.001 0.003 0.001
0.003 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.199 -0.109 0.045
-0.109 0.123 -0.051
0.045 -0.051 0.042
0.001 -0.003 0.001
-0.003 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.199 -0.109 -0.045
-0.109 0.123 0.051
-0.045 0.051 0.042
0.001 -0.003 -0.001
-0.003 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.199 0.109 -0.045
0.109 0.123 -0.051
-0.045 -0.051 0.042
0.001 0.003 -0.001
0.003 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.008 0.089 0.000
0.089 0.034 -0.014
0.000 -0.014 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 34 C
0.008 -0.090 0.000
-0.090 0.034 0.014
0.000 0.014 -0.057
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 35 C
0.008 -0.090 0.000
-0.090 0.034 -0.014
0.000 -0.014 -0.057
0.000 -0.002 0.000

-0.002 0.001 0.000
0.000 0.000 -0.001

atensor 36 C
0.008 0.090 0.000
0.090 0.034 0.014
0.000 0.014 -0.057
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 -0.001

atensor 37 C
0.024 0.080 0.031
0.080 0.005 0.014
0.031 0.014 -0.046
0.001 0.001 0.001
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 38 C
0.024 -0.080 0.031
-0.080 0.005 -0.014
0.031 -0.014 -0.046
0.001 -0.001 0.001
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 39 C
0.025 -0.080 -0.031
-0.080 0.005 0.014
-0.031 0.014 -0.046
0.001 -0.001 -0.001
-0.002 0.000 0.000
0.000 0.000 -0.001

atensor 40 C
0.024 0.080 -0.031
0.080 0.005 -0.014
-0.031 -0.014 -0.046
0.001 0.001 -0.001
0.002 0.000 0.000
0.000 0.000 -0.001

atensor 41 C
0.039 0.046 -0.007
0.046 0.040 0.019
-0.007 0.019 -0.026
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 -0.001

atensor 42 C
0.039 -0.046 -0.007
-0.046 0.040 -0.019
-0.007 -0.019 -0.026
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 -0.001

atensor 43 C
0.039 -0.046 0.007
-0.046 0.040 0.019
0.007 0.019 -0.026
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 -0.001

atensor 44 C
0.039 0.046 0.007
0.046 0.040 -0.019
0.007 -0.019 -0.026
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 -0.001

atensor 47 H
-0.579 0.354 0.010
0.354 0.695 0.253
0.010 0.253 -0.518
-0.014 0.003 0.000
0.009 0.020 0.005
0.000 0.002 -0.005

atensor 48 H
-0.579 -0.354 0.010
-0.354 0.695 -0.253
0.010 -0.253 -0.518
-0.014 -0.003 0.000
-0.009 0.020 -0.005
0.000 -0.002 -0.005

atensor 49 H
-0.579 -0.354 -0.010
-0.354 0.695 0.253
-0.010 0.253 -0.518
-0.014 -0.003 0.000
-0.009 0.020 0.005
0.000 0.002 -0.005

atensor 50 H
-0.579 0.354 -0.010
0.354 0.695 -0.253
-0.010 -0.253 -0.518
-0.014 0.003 0.000
0.009 0.020 -0.005
0.000 -0.002 -0.005

atensor 51 H
-0.100 0.647 -0.164
0.647 0.482 -0.270
-0.164 -0.270 -0.422
-0.002 0.013 -0.003
0.014 0.010 -0.006
-0.002 -0.003 -0.004

atensor 52 H
-0.100 -0.647 -0.164
-0.647 0.482 0.270
-0.164 0.270 -0.422
-0.002 -0.013 -0.003
-0.014 0.010 0.006
-0.002 0.003 -0.004

atensor 53 H
-0.100 -0.647 0.164
-0.647 0.482 -0.270
0.164 -0.270 -0.422
-0.002 -0.013 0.003
-0.014 0.010 -0.006
0.002 -0.003 -0.004

atensor 54 H
-0.100 0.647 0.164
0.647 0.482 0.270

0.164 0.270 -0.422
-0.002 0.013 0.003
0.014 0.010 0.006
0.002 0.003 -0.004

atensor 55 H
0.272 0.445 0.369
0.445 -0.114 0.229
0.369 0.229 -0.200
0.006 0.009 0.008
0.010 -0.002 0.005
0.004 0.003 -0.002

atensor 56 H
0.272 -0.445 0.369
-0.445 -0.114 -0.229
0.369 -0.229 -0.200
0.006 -0.009 0.008
-0.010 -0.002 -0.005
0.004 -0.003 -0.002

atensor 57 H
0.272 -0.445 -0.369
-0.445 -0.114 0.229
-0.369 0.229 -0.200
0.006 -0.009 -0.008
-0.010 -0.002 0.005
-0.004 0.003 -0.002

atensor 58 H
0.272 0.445 -0.369
0.445 -0.114 -0.229
-0.369 -0.229 -0.200
0.006 0.009 -0.008
0.010 -0.002 -0.005
-0.004 -0.003 -0.002

atensor 59 H
0.018 0.235 -0.044
0.235 0.156 -0.061
-0.044 -0.061 -0.140
0.000 0.005 -0.001
0.005 0.003 -0.001
-0.001 -0.001 -0.002

atensor 60 H
0.018 -0.235 -0.044
-0.235 0.156 0.061
-0.044 0.061 -0.140
0.000 -0.005 -0.001
-0.005 0.003 0.001
-0.001 0.001 -0.002

atensor 61 H
0.018 -0.235 0.044
-0.235 0.156 -0.061
0.044 -0.061 -0.140
0.000 -0.005 0.001
-0.005 0.003 -0.001
0.001 -0.001 -0.002

atensor 62 H
0.018 0.235 0.044
0.235 0.156 0.061
0.044 0.061 -0.140
0.000 0.005 0.001
0.005 0.003 0.001

0.001 0.001 -0.002

atensor 63 H
0.603 0.338 0.101
0.338 -0.767 -0.014
0.101 -0.014 -0.734
0.019 0.008 0.001
0.005 -0.014 0.001
0.001 0.001 -0.006

atensor 64 H
0.603 -0.338 0.101
-0.338 -0.767 0.014
0.101 0.014 -0.734
0.019 -0.008 0.001
-0.005 -0.014 -0.001
0.001 -0.001 -0.006

atensor 65 H
0.603 -0.338 -0.101
-0.338 -0.767 -0.014
-0.101 -0.014 -0.734
0.019 -0.008 -0.001
-0.005 -0.014 0.001
-0.001 0.001 -0.006

atensor 66 H
0.603 0.338 -0.101
0.338 -0.767 0.014
-0.101 0.014 -0.734
0.019 0.008 -0.001
0.005 -0.014 -0.001
-0.001 -0.001 -0.006

atensor 67 H
0.117 0.195 0.097
0.195 0.011 0.072
0.097 0.072 -0.096
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.117 -0.195 0.097
-0.195 0.011 -0.072
0.097 -0.072 -0.096
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.117 -0.195 -0.097
-0.195 0.011 0.072
-0.097 0.072 -0.096
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.117 0.195 -0.097
0.195 0.011 -0.072
-0.097 -0.072 -0.096
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H

0.040 0.169 0.012
0.169 0.043 0.017
0.012 0.017 -0.129
0.001 0.003 0.000
0.004 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.040 -0.169 0.012
-0.169 0.043 -0.017
0.012 -0.017 -0.129
0.001 -0.003 0.000
-0.004 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.040 -0.169 -0.012
-0.169 0.043 0.017
-0.012 0.017 -0.129
0.001 -0.003 0.000
-0.004 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.040 0.169 -0.012
0.169 0.043 -0.017
-0.012 -0.017 -0.129
0.001 0.003 0.000
0.004 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-220.279 -17.008 -2.449
-17.008 -306.310 -34.513
-2.449 -34.513 -81.941
262.057 -3.882 -0.981
-3.882 258.490 4.208
-0.981 4.208 222.882

orbtensor 2 C
-220.279 17.008 -2.449
17.008 -306.310 34.513
-2.449 34.513 -81.941
262.057 3.882 -0.981
3.882 258.490 -4.208
-0.981 -4.208 222.882

orbtensor 3 C
-220.279 17.008 2.449
17.008 -306.310 -34.513
2.449 -34.513 -81.941
262.057 3.882 0.981
3.882 258.490 4.208
0.981 4.208 222.882

orbtensor 4 C
-220.279 -17.008 2.449
-17.008 -306.310 34.513
2.449 34.513 -81.941
262.057 -3.882 0.981
-3.882 258.490 -4.208
0.981 -4.208 222.882

orbtensor 5 C
-276.149 -12.930 4.493
-12.930 -296.157 -25.633
4.493 -25.633 -94.366

271.220 2.189 -0.318
2.189 266.153 3.263
-0.318 3.263 229.184

orbtensor 6 C
-276.149 12.930 4.493
12.930 -296.157 25.633
4.493 25.633 -94.366
271.220 -2.189 -0.318
-2.189 266.153 -3.263
-0.318 -3.263 229.184

orbtensor 7 C
-276.149 12.930 -4.493
12.930 -296.157 -25.633
-4.493 -25.633 -94.366
271.220 -2.189 0.318
-2.189 266.153 3.263
0.318 3.263 229.184

orbtensor 8 C
-276.149 -12.930 -4.493
-12.930 -296.157 25.633
-4.493 25.633 -94.366
271.220 2.189 0.318
2.189 266.153 -3.263
0.318 -3.263 229.184

orbtensor 9 C
-251.665 -17.048 8.421
-17.048 -253.924 -10.729
8.421 -10.729 -64.990
262.869 0.696 -0.478
0.696 263.097 0.857
-0.478 0.857 217.410

orbtensor 10 C
-251.665 17.048 8.421
17.048 -253.924 10.729
8.421 10.729 -64.990
262.869 -0.696 -0.478
-0.696 263.097 -0.857
-0.478 -0.857 217.410

orbtensor 11 C
-251.665 17.048 -8.421
17.048 -253.924 -10.729
-8.421 -10.729 -64.990
262.869 -0.696 0.478
-0.696 263.097 0.857
0.478 0.857 217.410

orbtensor 12 C
-251.665 -17.048 -8.421
-17.048 -253.924 10.729
-8.421 10.729 -64.990
262.869 0.696 0.478
0.696 263.097 -0.857
0.478 -0.857 217.410

orbtensor 13 C
-291.128 -7.883 30.207
-7.883 -281.610 -14.780
30.207 -14.780 -84.759
266.707 1.958 -1.563
1.958 270.942 0.796
-1.563 0.796 229.234

orbtensor 14 C
-291.128 7.883 30.207
7.883 -281.609 14.780
30.207 14.780 -84.759
266.707 -1.958 -1.563
-1.958 270.942 -0.796
-1.563 -0.796 229.234

orbtensor 15 C
-291.128 7.883 -30.207
7.883 -281.610 -14.780
-30.207 -14.780 -84.759
266.707 -1.958 1.563
-1.958 270.942 0.796
1.563 0.796 229.234

orbtensor 16 C
-291.128 -7.883 -30.207
-7.883 -281.610 14.780
-30.207 14.780 -84.759
266.707 1.958 1.563
1.958 270.942 -0.796
1.563 -0.796 229.234

orbtensor 17 C
-220.595 -107.865 -56.469
-107.865 -218.924 58.733
-56.469 58.733 -210.910
254.082 14.331 9.932
14.331 254.107 -9.937
9.932 -9.937 250.001

orbtensor 18 C
-220.595 107.865 -56.469
107.865 -218.924 -58.733
-56.469 -58.733 -210.910
254.082 -14.331 9.932
-14.331 254.107 9.937
9.932 9.937 250.001

orbtensor 19 C
-220.595 107.865 56.469
107.865 -218.924 58.733
56.469 58.733 -210.911
254.082 -14.331 -9.932
-14.331 254.107 -9.937
-9.932 -9.937 250.001

orbtensor 20 C
-220.595 -107.865 56.469
-107.865 -218.924 -58.733
56.469 -58.733 -210.910
254.082 14.331 -9.932
14.331 254.107 9.937
-9.932 9.937 250.001

orbtensor 23 C
-199.879 69.796 90.822
69.796 -165.690 49.516
90.822 49.516 -256.311
247.005 -14.817 -6.165
-14.817 250.223 -13.245
-6.165 -13.245 249.274

orbtensor 24 C
-199.879 -69.796 90.822

-69.796	-165.690	-49.516
90.822	-49.516	-256.311
247.005	14.817	-6.165
14.817	250.223	13.245
-6.165	13.245	249.274

orbtensor 25 C

-300.121	-14.198	36.296
-14.198	-218.471	13.409
36.296	13.409	-81.385
259.146	-4.032	-3.577
-4.032	261.259	1.058
-3.577	1.058	222.229

orbtensor 26 C

-300.121	14.198	36.296
14.198	-218.471	-13.409
36.296	-13.409	-81.385
259.146	4.032	-3.577
4.032	261.259	-1.058
-3.577	-1.058	222.229

orbtensor 27 C

-300.121	14.198	-36.296
14.198	-218.471	13.409
-36.296	13.409	-81.385
259.146	4.032	3.577
4.032	261.259	1.058
3.577	1.058	222.229

orbtensor 28 C

-300.121	-14.198	-36.296
-14.198	-218.471	-13.409
-36.296	-13.409	-81.385
259.146	-4.032	3.577
-4.032	261.259	-1.058
3.577	-1.058	222.229

orbtensor 29 C

-164.859	-67.527	-50.947
-67.527	-194.751	89.604
-50.947	89.604	-257.150
249.885	14.884	13.269
14.884	246.551	-6.420
13.269	-6.420	248.885

orbtensor 30 C

-164.859	67.528	-50.947
67.528	-194.751	-89.604
-50.947	-89.604	-257.150
249.885	-14.884	13.269
-14.884	246.551	6.420
13.269	6.420	248.885

orbtensor 31 C

-164.859	67.528	50.947
67.528	-194.751	89.604
50.947	89.604	-257.150
249.885	-14.884	-13.269
-14.884	246.551	-6.420
-13.269	-6.420	248.885

orbtensor 32 C

-164.859	-67.528	50.947
-67.528	-194.751	-89.604
50.947	-89.604	-257.150
249.885	14.884	-13.269

14.884 246.551 6.420
-13.269 6.420 248.885

orbtensor 33 C
-153.822 -70.165 -47.772
-70.165 -193.271 99.334
-47.772 99.334 -227.266
246.177 15.540 10.656
15.540 243.958 -9.555
10.656 -9.555 245.361

orbtensor 34 C
-153.822 70.165 -47.772
70.165 -193.270 -99.334
-47.772 -99.334 -227.266
246.177 -15.540 10.656
-15.540 243.958 9.555
10.656 9.555 245.361

orbtensor 35 C
-153.822 70.165 47.772
70.165 -193.271 99.334
47.772 99.334 -227.266
246.177 -15.540 -10.656
-15.540 243.958 -9.555
-10.656 -9.555 245.361

orbtensor 36 C
-153.822 -70.165 47.772
-70.165 -193.271 -99.334
47.772 -99.334 -227.266
246.177 15.540 -10.656
15.540 243.958 9.555
-10.656 9.555 245.361

orbtensor 37 C
-196.654 -72.361 -98.843
-72.361 -153.080 45.486
-98.843 45.486 -224.648
244.442 15.426 9.371
15.426 246.202 -10.751
9.371 -10.751 245.650

orbtensor 38 C
-196.654 72.360 -98.843
72.360 -153.080 -45.486
-98.843 -45.486 -224.648
244.442 -15.426 9.371
-15.426 246.202 10.751
9.371 10.751 245.650

orbtensor 39 C
-196.654 72.361 98.843
72.361 -153.080 45.486
98.843 45.486 -224.648
244.442 -15.426 -9.371
-15.426 246.202 -10.751
-9.371 -10.751 245.650

orbtensor 40 C
-196.654 -72.360 98.843
-72.360 -153.080 -45.486
98.843 -45.486 -224.648
244.442 15.426 -9.371
15.426 246.202 10.751
-9.371 10.751 245.650

orbtensor 41 C
-204.687 -114.172 -52.316
-114.172 -205.364 55.459
-52.316 55.459 -176.073
245.935 12.114 10.806
12.114 245.669 -10.929
10.806 -10.929 250.026

orbtensor 42 C
-204.687 114.172 -52.316
114.172 -205.364 -55.459
-52.316 -55.459 -176.073
245.935 -12.114 10.806
-12.114 245.669 10.929
10.806 10.929 250.026

orbtensor 43 C
-204.687 114.172 52.316
114.172 -205.364 55.459
52.316 55.459 -176.073
245.935 -12.114 -10.806
-12.114 245.669 -10.929
-10.806 -10.929 250.026

orbtensor 44 C
-204.687 -114.172 52.316
-114.172 -205.364 -55.459
52.316 -55.459 -176.073
245.935 12.114 -10.806
12.114 245.669 10.929
-10.806 10.929 250.026

orbtensor 47 H
-3.550 -8.483 -1.731
-8.483 -15.155 -1.843
-1.731 -1.843 -5.756
35.311 4.789 -0.715
4.789 35.623 2.409
-0.715 2.409 18.588

orbtensor 48 H
-3.550 8.483 -1.731
8.483 -15.155 1.843
-1.731 1.843 -5.756
35.311 -4.789 -0.715
-4.789 35.623 -2.409
-0.715 -2.409 18.588

orbtensor 49 H
-3.550 8.483 1.731
8.483 -15.155 -1.843
1.731 -1.843 -5.756
35.311 -4.789 0.715
-4.789 35.623 2.409
0.715 2.409 18.588

orbtensor 50 H
-3.550 -8.483 1.731
-8.483 -15.155 1.843
1.731 1.843 -5.756
35.311 4.789 0.715
4.789 35.623 -2.409
0.715 -2.409 18.588

orbtensor 51 H
-8.832 -2.307 -9.751
-2.307 -3.107 -2.143

-9.751	-2.143	-13.086
32.431	4.564	5.557
4.564	27.200	-3.797
5.557	-3.797	33.440

orbtensor 52 H

-8.832	2.307	-9.751
2.307	-3.107	2.143
-9.751	2.143	-13.086
32.431	-4.564	5.557
-4.564	27.200	3.797
5.557	3.797	33.440

orbtensor 53 H

-8.832	2.307	9.751
2.307	-3.107	-2.143
9.751	-2.143	-13.086
32.431	-4.564	-5.557
-4.564	27.200	-3.797
-5.557	-3.797	33.440

orbtensor 54 H

-8.832	-2.307	9.751
-2.307	-3.107	2.143
9.751	2.143	-13.086
32.431	4.564	-5.557
4.564	27.200	3.797
-5.557	3.797	33.440

orbtensor 55 H

-2.834	-1.689	1.501
-1.689	-8.458	9.618
1.501	9.618	-14.503
27.190	4.058	4.157
4.058	32.317	-5.469
4.157	-5.469	34.097

orbtensor 56 H

-2.834	1.689	1.501
1.689	-8.458	-9.618
1.501	-9.618	-14.503
27.190	-4.058	4.157
-4.058	32.317	5.469
4.157	5.469	34.097

orbtensor 57 H

-2.834	1.689	-1.501
1.689	-8.458	9.618
-1.501	9.618	-14.503
27.190	-4.058	-4.157
-4.058	32.317	-5.469
-4.157	-5.469	34.097

orbtensor 58 H

-2.834	-1.689	-1.501
-1.689	-8.458	-9.618
-1.501	-9.618	-14.503
27.190	4.058	-4.157
4.058	32.317	5.469
-4.157	5.469	34.097

orbtensor 59 H

-1.984	-1.317	0.504
-1.317	-9.426	7.814
0.504	7.814	-12.523
27.004	3.714	0.805
3.714	32.778	-9.064

0.805 -9.064 33.955

orbtensor 60 H

-1.984 1.317 0.504
1.317 -9.426 -7.814
0.504 -7.814 -12.523
27.004 -3.714 0.805
-3.714 32.778 9.064
0.805 9.064 33.955

orbtensor 61 H

-1.984 1.317 -0.504
1.317 -9.426 7.814
-0.504 7.814 -12.523
27.004 -3.714 -0.805
-3.714 32.778 -9.064
-0.805 -9.064 33.955

orbtensor 62 H

-1.984 -1.317 -0.504
-1.317 -9.426 -7.814
-0.504 -7.814 -12.523
27.004 3.714 -0.805
3.714 32.778 9.064
-0.805 9.064 33.955

orbtensor 63 H

-15.025 -8.335 1.599
-8.335 -3.411 1.911
1.599 1.911 -5.806
36.281 4.838 -1.963
4.838 35.254 0.707
-1.963 0.707 18.403

orbtensor 64 H

-15.025 8.335 1.599
8.335 -3.411 -1.911
1.599 -1.911 -5.806
36.281 -4.838 -1.963
-4.838 35.254 -0.707
-1.963 -0.707 18.403

orbtensor 65 H

-15.025 8.335 -1.599
8.335 -3.411 1.911
-1.599 1.911 -5.806
36.281 -4.838 1.963
-4.838 35.254 0.707
1.963 0.707 18.403

orbtensor 66 H

-15.025 -8.335 -1.599
-8.335 -3.411 -1.911
-1.599 -1.911 -5.806
36.281 4.838 1.963
4.838 35.254 -0.707
1.963 -0.707 18.403

orbtensor 67 H

-9.802 -1.622 -7.899
-1.622 -2.081 -0.877
-7.899 -0.877 -12.231
33.186 3.943 9.037
3.943 27.082 -0.564
9.037 -0.564 33.629

orbtensor 68 H

```
-9.802    1.622   -7.899
1.622   -2.081    0.877
-7.899    0.877  -12.231
33.186   -3.943    9.037
-3.943   27.082    0.564
9.037    0.564   33.629
```

orbtensor 69 H

```
-9.802    1.622    7.899
1.622   -2.081   -0.877
7.899   -0.877  -12.231
33.186   -3.943   -9.037
-3.943   27.082   -0.564
-9.037   -0.564   33.629
```

orbtensor 70 H

```
-9.802   -1.622    7.899
-1.622   -2.081    0.877
7.899    0.877  -12.231
33.186    3.943   -9.037
3.943   27.082    0.564
-9.037    0.564   33.629
```

orbtensor 71 H

```
-10.546   -9.044    0.312
-9.044  -10.801    0.131
0.312    0.131   -2.987
33.758    9.676    1.579
9.676   33.916   -2.017
1.579   -2.017   26.549
```

orbtensor 72 H

```
-10.546    9.044    0.312
9.044  -10.801   -0.131
0.312   -0.131   -2.987
33.758   -9.676    1.579
-9.676   33.916    2.017
1.579    2.017   26.549
```

orbtensor 73 H

```
-10.546    9.044   -0.312
9.044  -10.801    0.131
-0.312    0.131   -2.987
33.758   -9.676   -1.579
-9.676   33.916   -2.017
-1.579   -2.017   26.549
```

orbtensor 74 H

```
-10.546   -9.044   -0.312
-9.044  -10.801   -0.131
-0.312   -0.131   -2.987
33.758    9.676   -1.579
9.676   33.916    2.017
-1.579    2.017   26.549
```

gtensor (ppt)

```
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
0.0 0.0 0.0
```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4253	44.96633	220.38956	0.00000	220.38956	265.35589
2	C	-0.4253	44.96633	220.38956	0.00000	220.38956	265.35589
3	C	-0.4253	44.96633	220.38956	0.00000	220.38956	265.35589
4	C	-0.4253	44.96633	220.38956	0.00000	220.38956	265.35589
5	C	-1.2133	33.29500	628.69749	0.00000	628.69749	661.99249
6	C	-1.2133	33.29500	628.69749	0.00000	628.69749	661.99249
7	C	-1.2133	33.29500	628.69749	0.00000	628.69749	661.99249
8	C	-1.2133	33.29500	628.69749	0.00000	628.69749	661.99249
9	C	0.4370	57.59900	-226.43473	0.00000	-226.43473	-168.83573
10	C	0.4370	57.59900	-226.43473	0.00000	-226.43473	-168.83573
11	C	0.4370	57.59900	-226.43473	0.00000	-226.43473	-168.83573
12	C	0.4370	57.59900	-226.43473	0.00000	-226.43473	-168.83573
13	C	-0.9920	36.46200	514.01201	0.00000	514.01201	550.47401
14	C	-0.9923	36.46233	514.18473	0.00000	514.18473	550.64707
15	C	-0.9923	36.46200	514.18473	0.00000	514.18473	550.64673
16	C	-0.9923	36.46200	514.18473	0.00000	514.18473	550.64673
17	C	-0.0740	35.92033	38.34364	0.00000	38.34364	74.26397
18	C	-0.0740	35.92033	38.34364	0.00000	38.34364	74.26397
19	C	-0.0740	35.92000	38.34364	0.00000	38.34364	74.26364
20	C	-0.0740	35.92033	38.34364	0.00000	38.34364	74.26397
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1393	41.54067	-72.19658	0.00000	-72.19658	-30.65591
24	C	0.1393	41.54067	-72.19658	0.00000	-72.19658	-30.65591
25	C	-0.6717	47.55233	348.02897	0.00000	348.02897	395.58130
26	C	-0.6717	47.55233	348.02897	0.00000	348.02897	395.58130
27	C	-0.6717	47.55233	348.02897	0.00000	348.02897	395.58130
28	C	-0.6717	47.55233	348.02897	0.00000	348.02897	395.58130
29	C	0.1213	42.85367	-62.86975	0.00000	-62.86975	-20.01608
30	C	0.1213	42.85367	-62.86975	0.00000	-62.86975	-20.01608
31	C	0.1213	42.85367	-62.86975	0.00000	-62.86975	-20.01608
32	C	0.1213	42.85367	-62.86975	0.00000	-62.86975	-20.01608
33	C	-0.0050	53.71233	2.59079	0.00000	2.59079	56.30312
34	C	-0.0050	53.71267	2.59079	0.00000	2.59079	56.30345
35	C	-0.0050	53.71233	2.59079	0.00000	2.59079	56.30312
36	C	-0.0050	53.71233	2.59079	0.00000	2.59079	56.30312
A Average		-1.1028	34.87854	571.41952	0.00000	571.41952	606.29806
B Average		-0.5485	46.25933	284.20926	0.00000	284.20926	330.46860
M Average		0.4370	57.59900	-226.43473	0.00000	-226.43473	-168.83573

FeL5-saddled-HS-STO-PBE0-Full-Finite

Temperature: 303

Spin: 2.5

atensor 1 C

0.687 0.061 0.014
0.061 1.476 0.115
0.014 0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C

0.687 -0.061 0.014
-0.061 1.476 -0.115
0.014 -0.115 0.766
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C
0.687 -0.061 -0.014
-0.061 1.476 0.115
-0.014 0.115 0.766
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.687 0.061 -0.014
0.061 1.476 -0.115
-0.014 -0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.790 0.802 0.105
0.802 1.951 0.315
0.105 0.315 0.010
-0.003 0.005 0.000
0.007 0.005 0.001
0.000 0.001 0.002

atensor 6 C
0.790 -0.802 0.105
-0.802 1.951 -0.315
0.105 -0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 7 C
0.790 -0.802 -0.105
-0.802 1.951 0.315
-0.105 0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 0.001
0.000 0.001 0.002

atensor 8 C
0.790 0.802 -0.105
0.802 1.951 -0.315
-0.105 -0.315 0.010
-0.003 0.005 0.000
0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 9 C
0.207 0.595 0.154
0.595 0.223 0.142
0.154 0.142 0.407
-0.001 -0.002 0.001
-0.004 -0.002 0.001
0.001 0.000 0.000

atensor 10 C
0.207 -0.595 0.154
-0.595 0.223 -0.142
0.154 -0.142 0.407
-0.001 0.002 0.001
0.004 -0.002 -0.001
0.001 0.000 0.000

atensor 11 C
0.207 -0.595 -0.154
-0.595 0.223 0.142

-0.154 0.142 0.407
-0.001 0.002 -0.001
0.004 -0.002 0.001
-0.001 0.000 0.000

atensor 12 C
0.207 0.595 -0.154
0.595 0.223 -0.142
-0.154 -0.142 0.407
-0.001 -0.002 -0.001
-0.004 -0.002 -0.001
-0.001 0.000 0.000

atensor 13 C
1.511 0.799 0.149
0.799 0.400 0.042
0.149 0.042 -0.420
0.003 0.006 0.001
0.005 -0.002 0.000
0.001 -0.002 0.001

atensor 14 C
1.511 -0.799 0.149
-0.799 0.400 -0.042
0.149 -0.042 -0.420
0.003 -0.006 0.001
-0.005 -0.002 0.000
0.001 0.002 0.001

atensor 15 C
1.511 -0.799 -0.149
-0.799 0.400 0.042
-0.149 0.042 -0.420
0.003 -0.006 -0.001
-0.005 -0.002 0.000
-0.001 -0.002 0.001

atensor 16 C
1.510 0.799 -0.149
0.799 0.400 -0.042
-0.149 -0.042 -0.420
0.003 0.006 -0.001
0.005 -0.002 0.000
-0.001 0.002 0.001

atensor 17 C
-0.112 0.242 0.049
0.242 -0.105 0.014
0.049 0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.112 -0.242 0.049
-0.242 -0.105 -0.014
0.049 -0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.112 -0.242 -0.049
-0.242 -0.105 0.014
-0.049 0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000

```
0.000 0.000 0.000

atensor 20 C
-0.112 0.242 -0.049
0.242 -0.105 -0.014
-0.049 -0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.198 -0.132 0.028
-0.132 0.310 -0.017
0.028 -0.017 0.076
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.198 0.132 0.028
0.132 0.310 0.017
0.028 0.017 0.076
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.639 0.086 -0.011
0.086 0.799 0.023
-0.011 0.023 0.831
0.002 -0.001 0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 26 C
1.639 -0.086 -0.011
-0.086 0.799 -0.023
-0.011 -0.023 0.831
0.002 0.001 0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 27 C
1.639 -0.086 0.011
-0.086 0.799 0.023
0.011 0.023 0.831
0.002 0.001 -0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 28 C
1.639 0.086 0.011
0.086 0.799 -0.023
0.011 -0.023 0.831
0.002 -0.001 -0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 29 C
0.282 0.110 0.044
0.110 0.190 0.053
0.044 0.053 0.095
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
```

0.282 -0.110 0.044
-0.110 0.190 -0.053
0.044 -0.053 0.095
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.282 -0.110 -0.044
-0.110 0.190 0.053
-0.044 0.053 0.095
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.282 0.110 -0.044
0.110 0.190 -0.053
-0.044 -0.053 0.095
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.013 0.093 -0.001
0.093 0.041 -0.019
-0.001 -0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.013 -0.093 -0.001
-0.093 0.041 0.019
-0.001 0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.013 -0.093 0.001
-0.093 0.041 -0.019
0.001 -0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.013 0.093 0.001
0.093 0.041 0.019
0.001 0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-219.798 -16.527 0.247
-16.527 -304.533 -32.628
0.247 -32.628 -81.387
261.916 -3.867 -0.977
-3.867 258.311 4.277
-0.977 4.277 222.786

orbtensor 2 C
-219.798 16.527 0.247
16.527 -304.533 32.628
0.247 32.628 -81.387

261.916 3.867 -0.977
3.867 258.311 -4.277
-0.977 -4.277 222.786

orbtensor 3 C
-219.798 16.527 -0.247
16.527 -304.533 -32.628
-0.247 -32.628 -81.387
261.916 3.867 0.977
3.867 258.310 4.277
0.977 4.277 222.786

orbtensor 4 C
-219.798 -16.527 -0.247
-16.527 -304.533 32.628
-0.247 32.628 -81.387
261.916 -3.867 0.977
-3.867 258.310 -4.277
0.977 -4.277 222.786

orbtensor 5 C
-277.637 -8.681 1.112
-8.681 -296.230 -21.902
1.112 -21.902 -106.798
270.796 2.396 -0.261
2.396 265.805 3.262
-0.261 3.262 228.473

orbtensor 6 C
-277.637 8.681 1.112
8.681 -296.230 21.902
1.112 21.902 -106.798
270.796 -2.396 -0.261
-2.396 265.805 -3.262
-0.261 -3.262 228.473

orbtensor 7 C
-277.637 8.681 -1.112
8.681 -296.230 -21.902
-1.112 -21.902 -106.798
270.796 -2.396 0.261
-2.396 265.805 3.262
0.261 3.262 228.473

orbtensor 8 C
-277.637 -8.681 -1.112
-8.681 -296.230 21.902
-1.112 21.902 -106.798
270.795 2.396 0.261
2.396 265.805 -3.262
0.261 -3.262 228.472

orbtensor 9 C
-249.491 -12.396 9.928
-12.396 -252.178 -11.080
9.928 -11.080 -66.308
262.720 0.698 -0.426
0.698 262.961 0.841
-0.426 0.841 217.221

orbtensor 10 C
-249.491 12.396 9.928
12.396 -252.178 11.080
9.928 11.080 -66.308
262.720 -0.698 -0.426
-0.698 262.961 -0.841
-0.426 -0.841 217.221

orbtensor 11 C
-249.491 12.396 -9.928
12.396 -252.177 -11.080
-9.928 -11.080 -66.308
262.720 -0.698 0.426
-0.698 262.961 0.841
0.426 0.841 217.221

orbtensor 12 C
-249.491 -12.396 -9.928
-12.396 -252.178 11.080
-9.928 11.080 -66.309
262.720 0.698 0.426
0.698 262.961 -0.841
0.426 -0.841 217.221

orbtensor 13 C
-287.722 -4.323 23.246
-4.323 -284.314 -1.604
23.246 -1.604 -96.264
266.346 2.106 -1.575
2.106 270.495 0.787
-1.575 0.787 228.491

orbtensor 14 C
-287.722 4.323 23.246
4.323 -284.314 1.604
23.246 1.604 -96.264
266.346 -2.106 -1.575
-2.106 270.495 -0.787
-1.575 -0.787 228.490

orbtensor 15 C
-287.722 4.323 -23.246
4.323 -284.314 -1.604
-23.246 -1.604 -96.264
266.346 -2.106 1.575
-2.106 270.495 0.787
1.575 0.787 228.491

orbtensor 16 C
-287.722 -4.323 -23.246
-4.323 -284.314 1.604
-23.246 1.604 -96.264
266.346 2.106 1.575
2.106 270.495 -0.787
1.575 -0.787 228.490

orbtensor 17 C
-220.425 -107.042 -56.328
-107.042 -218.711 58.919
-56.328 58.919 -212.040
253.905 14.332 9.928
14.332 253.937 -9.939
9.928 -9.939 249.814

orbtensor 18 C
-220.425 107.042 -56.328
107.042 -218.711 -58.919
-56.328 -58.919 -212.039
253.905 -14.332 9.928
-14.332 253.937 9.939
9.928 9.939 249.814

orbtensor 19 C
-220.425 107.042 56.328

107.042	-218.711	58.919
56.328	58.919	-212.039
253.905	-14.332	-9.928
-14.332	253.937	-9.939
-9.928	-9.939	249.814

orbtensor 20 C

-220.425	-107.042	56.328
-107.042	-218.711	-58.919
56.328	-58.919	-212.039
253.905	14.332	-9.928
14.332	253.937	9.939
-9.928	9.939	249.814

orbtensor 23 C

-199.906	69.053	90.890
69.053	-165.240	49.179
90.890	49.179	-256.951
246.835	-14.813	-6.186
-14.813	250.029	-13.239
-6.186	-13.239	249.087

orbtensor 24 C

-199.906	-69.053	90.890
-69.053	-165.240	-49.179
90.890	-49.179	-256.951
246.835	14.813	-6.186
14.813	250.029	13.239
-6.186	13.239	249.087

orbtensor 25 C

-298.442	-13.808	34.429
-13.808	-218.228	5.976
34.429	5.976	-82.159
259.034	-4.004	-3.491
-4.004	261.073	1.044
-3.491	1.044	222.064

orbtensor 26 C

-298.442	13.808	34.428
13.808	-218.228	-5.976
34.428	-5.976	-82.159
259.034	4.004	-3.491
4.004	261.073	-1.044
-3.491	-1.044	222.063

orbtensor 27 C

-298.442	13.808	-34.428
13.808	-218.228	5.976
-34.428	5.976	-82.159
259.034	4.004	3.491
4.004	261.073	1.044
3.491	1.044	222.064

orbtensor 28 C

-298.442	-13.808	-34.429
-13.808	-218.228	-5.976
-34.429	-5.976	-82.159
259.034	-4.004	3.491
-4.004	261.073	-1.044
3.491	-1.044	222.063

orbtensor 29 C

-164.718	-67.087	-50.667
-67.087	-194.781	89.679
-50.667	89.679	-257.645
249.703	14.878	13.275

14.878 246.374 -6.421
13.275 -6.421 248.699

orbtensor 30 C
-164.718 67.087 -50.667
67.087 -194.781 -89.679
-50.667 -89.679 -257.645
249.703 -14.878 13.275
-14.878 246.374 6.421
13.275 6.421 248.699

orbtensor 31 C
-164.718 67.087 50.667
67.087 -194.781 89.679
50.667 89.679 -257.645
249.703 -14.878 -13.275
-14.878 246.374 -6.421
-13.275 -6.421 248.699

orbtensor 32 C
-164.718 -67.087 50.667
-67.087 -194.781 -89.679
50.667 -89.679 -257.645
249.703 14.878 -13.275
14.878 246.374 6.421
-13.275 6.421 248.699

orbtensor 33 C
-153.672 -69.730 -47.690
-69.730 -193.105 99.196
-47.690 99.196 -227.627
246.002 15.537 10.651
15.537 243.801 -9.560
10.651 -9.560 245.187

orbtensor 34 C
-153.671 69.730 -47.690
69.730 -193.105 -99.195
-47.690 -99.195 -227.627
246.002 -15.537 10.651
-15.537 243.801 9.560
10.651 9.560 245.187

orbtensor 35 C
-153.672 69.730 47.690
69.730 -193.105 99.196
47.690 99.196 -227.627
246.002 -15.537 -10.651
-15.537 243.801 -9.560
-10.651 -9.560 245.187

orbtensor 36 C
-153.672 -69.730 47.690
-69.730 -193.105 -99.195
47.690 -99.195 -227.627
246.002 15.537 -10.651
15.537 243.801 9.560
-10.651 9.560 245.187

gtensor (ppt)
-0.175 0.000 0.000
0.000 -0.177 0.000
0.000 0.000 -0.167
13.608 0.000 0.000
0.000 15.405 0.000
0.000 0.000 4.418
zfstensor (cm-1)

```

-0.335571    0.000004    0.000001
0.000004    -0.437059    -0.000068
0.000001    -0.000068    1.385620

```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9737	45.76500	-1183.65137	-3.08262	-1186.73400	-1140.96900
2	C	0.9737	45.76500	-1183.65137	-3.08244	-1186.73381	-1140.96881
3	C	0.9737	45.76467	-1183.65137	-3.08263	-1186.73400	-1140.96934
4	C	0.9737	45.76467	-1183.65137	-3.08243	-1186.73380	-1140.96914
5	C	0.9183	28.13633	-1116.38464	-12.23946	-1128.62410	-1100.48776
6	C	0.9183	28.13633	-1116.38464	-12.23901	-1128.62365	-1100.48732
7	C	0.9183	28.13633	-1116.38464	-12.23954	-1128.62418	-1100.48785
8	C	0.9183	28.13567	-1116.38464	-12.23893	-1128.62357	-1100.48791
9	C	0.2780	58.30833	-337.95455	1.65151	-336.30304	-277.99471
10	C	0.2780	58.30833	-337.95455	1.65169	-336.30286	-277.99453
11	C	0.2780	58.30867	-337.95455	1.65145	-336.30310	-277.99444
12	C	0.2780	58.30800	-337.95455	1.65174	-336.30281	-277.99481
13	C	0.4977	32.34400	-604.99538	-11.23289	-616.22827	-583.88427
14	C	0.4977	32.34367	-604.99538	-11.23290	-616.22828	-583.88462
15	C	0.4977	32.34400	-604.99538	-11.23298	-616.22835	-583.88435
16	C	0.4973	32.34367	-604.59016	-11.22904	-615.81920	-583.47553
17	C	-0.1840	35.49333	223.68215	-1.95787	221.72428	257.21761
18	C	-0.1840	35.49367	223.68215	-1.95787	221.72428	257.21794
19	C	-0.1840	35.49367	223.68215	-1.95790	221.72425	257.21792
20	C	-0.1840	35.49367	223.68215	-1.95785	221.72430	257.21797
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1950	41.28467	-237.05445	-1.58680	-238.64125	-197.35658
24	C	0.1950	41.28467	-237.05445	-1.58681	-238.64126	-197.35660
25	C	1.0860	47.78067	-1320.21095	-2.86667	-1323.07761	-1275.29695
26	C	1.0860	47.78033	-1320.21095	-2.86664	-1323.07758	-1275.29725
27	C	1.0860	47.78067	-1320.21095	-2.86668	-1323.07762	-1275.29696
28	C	1.0860	47.78033	-1320.21095	-2.86663	-1323.07757	-1275.29724
29	C	0.1890	42.54400	-229.76047	-1.16311	-230.92358	-188.37958
30	C	0.1890	42.54400	-229.76047	-1.16303	-230.92350	-188.37950
31	C	0.1890	42.54400	-229.76047	-1.16312	-230.92359	-188.37959
32	C	0.1890	42.54400	-229.76047	-1.16302	-230.92349	-188.37949
33	C	0.0003	53.52867	-0.40522	-0.69986	-1.10508	52.42358
34	C	0.0003	53.52900	-0.40522	-0.69990	-1.10512	52.42388
35	C	0.0003	53.52867	-0.40522	-0.69987	-1.10509	52.42357
36	C	0.0003	53.52867	-0.40522	-0.69989	-1.10512	52.42355
A Average		0.7080	30.24000	-860.63936	-11.73559	-872.37495	-842.13495
B Average		1.0298	46.77267	-1251.93116	-2.97459	-1254.90575	-1208.13308
M Average		0.2780	58.30833	-337.95455	1.65160	-336.30295	-277.99462

=====
FeL5-saddled-HS-STO-PBE0-Full-ORCA

Temperature: 303

Spin: 2.5

atensor 1 C

```

0.687 0.061 0.014
0.061 1.476 0.115
0.014 0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

```

atensor 2 C
0.687 -0.061 0.014
-0.061 1.476 -0.115
0.014 -0.115 0.766
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C
0.687 -0.061 -0.014
-0.061 1.476 0.115
-0.014 0.115 0.766
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.687 0.061 -0.014
0.061 1.476 -0.115
-0.014 -0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.790 0.802 0.105
0.802 1.951 0.315
0.105 0.315 0.010
-0.003 0.005 0.000
0.007 0.005 0.001
0.000 0.001 0.002

atensor 6 C
0.790 -0.802 0.105
-0.802 1.951 -0.315
0.105 -0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 7 C
0.790 -0.802 -0.105
-0.802 1.951 0.315
-0.105 0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 0.001
0.000 0.001 0.002

atensor 8 C
0.790 0.802 -0.105
0.802 1.951 -0.315
-0.105 -0.315 0.010
-0.003 0.005 0.000
0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 9 C
0.207 0.595 0.154
0.595 0.224 0.142
0.154 0.142 0.408
-0.001 -0.002 0.001
-0.004 -0.002 0.001
0.001 0.000 0.000

atensor 10 C
0.207 -0.595 0.154
-0.595 0.224 -0.142

0.154 -0.142 0.408
-0.001 0.002 0.001
0.004 -0.002 -0.001
0.001 0.000 0.000

atensor 11 C
0.207 -0.595 -0.154
-0.595 0.224 0.142
-0.154 0.142 0.408
-0.001 0.002 -0.001
0.004 -0.002 0.001
-0.001 0.000 0.000

atensor 12 C
0.207 0.595 -0.154
0.595 0.224 -0.142
-0.154 -0.142 0.408
-0.001 -0.002 -0.001
-0.004 -0.002 -0.001
-0.001 0.000 0.000

atensor 13 C
1.511 0.799 0.149
0.799 0.400 0.042
0.149 0.042 -0.420
0.003 0.006 0.001
0.005 -0.002 0.000
0.001 -0.002 0.001

atensor 14 C
1.511 -0.799 0.149
-0.799 0.400 -0.042
0.149 -0.042 -0.420
0.003 -0.006 0.001
-0.005 -0.002 0.000
0.001 0.002 0.001

atensor 15 C
1.511 -0.799 -0.149
-0.799 0.400 0.042
-0.149 0.042 -0.420
0.003 -0.006 -0.001
-0.005 -0.002 0.000
-0.001 -0.002 0.001

atensor 16 C
1.511 0.799 -0.149
0.799 0.400 -0.042
-0.149 -0.042 -0.420
0.003 0.006 -0.001
0.005 -0.002 0.000
-0.001 0.002 0.001

atensor 17 C
-0.112 0.242 0.049
0.242 -0.105 0.014
0.049 0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.112 -0.242 0.049
-0.242 -0.105 -0.014
0.049 -0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000

0.000 0.000 0.000

atensor 19 C
-0.112 -0.242 -0.049
-0.242 -0.105 0.014
-0.049 0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.112 0.242 -0.049
0.242 -0.105 -0.014
-0.049 -0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.199 -0.132 0.028
-0.132 0.311 -0.017
0.028 -0.017 0.076
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.199 0.132 0.028
0.132 0.311 0.017
0.028 0.017 0.076
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.639 0.086 -0.011
0.086 0.799 0.023
-0.011 0.023 0.831
0.002 -0.001 0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 26 C
1.639 -0.086 -0.011
-0.086 0.799 -0.023
-0.011 -0.023 0.831
0.002 0.001 0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 27 C
1.639 -0.086 0.011
-0.086 0.799 0.023
0.011 0.023 0.831
0.002 0.001 -0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 28 C
1.639 0.086 0.011
0.086 0.799 -0.023
0.011 -0.023 0.831
0.002 -0.001 -0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 29 C

0.282 0.110 0.044
0.110 0.190 0.053
0.044 0.053 0.095
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.282 -0.110 0.044
-0.110 0.190 -0.053
0.044 -0.053 0.095
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.282 -0.110 -0.044
-0.110 0.190 0.053
-0.044 0.053 0.095
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.282 0.110 -0.044
0.110 0.190 -0.053
-0.044 -0.053 0.095
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.013 0.093 -0.001
0.093 0.041 -0.019
-0.001 -0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.013 -0.093 -0.001
-0.093 0.041 0.019
-0.001 0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.013 -0.093 0.001
-0.093 0.041 -0.019
0.001 -0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.013 0.093 0.001
0.093 0.041 0.019
0.001 0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.033 0.085 0.032
0.085 0.010 0.012
0.032 0.012 -0.045

0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.033 -0.085 0.032
-0.085 0.011 -0.012
0.032 -0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.033 -0.085 -0.032
-0.085 0.011 0.012
-0.032 0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.033 0.085 -0.032
0.085 0.011 -0.012
-0.032 -0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.043 0.045 -0.010
0.045 0.045 0.020
-0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.043 -0.045 -0.010
-0.045 0.045 -0.020
-0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.043 -0.045 0.010
-0.045 0.045 0.020
0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.043 0.045 0.010
0.045 0.045 -0.020
0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.176 0.408 0.068
0.408 1.085 0.236
0.068 0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 0.002
0.000 0.000 -0.001

atensor 48 H
-0.176 -0.408 0.068
-0.408 1.085 -0.236
0.068 -0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 49 H
-0.176 -0.408 -0.068
-0.408 1.085 0.236
-0.068 0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 0.002
0.000 0.000 -0.001

atensor 50 H
-0.176 0.408 -0.068
0.408 1.085 -0.236
-0.068 -0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 51 H
-0.112 0.622 -0.191
0.622 0.452 -0.314
-0.191 -0.314 -0.411
-0.001 0.005 -0.001
0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 52 H
-0.112 -0.622 -0.191
-0.622 0.452 0.314
-0.191 0.314 -0.411
-0.001 -0.005 -0.001
-0.005 0.004 0.002
0.000 0.001 -0.001

atensor 53 H
-0.112 -0.622 0.191
-0.622 0.452 -0.314
0.191 -0.314 -0.411
-0.001 -0.005 0.001
-0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 54 H
-0.112 0.622 0.191
0.622 0.452 0.314
0.191 0.314 -0.411
-0.001 0.005 0.001
0.005 0.004 0.002
0.000 0.001 -0.001

atensor 55 H
0.262 0.457 0.389
0.457 -0.111 0.250
0.389 0.250 -0.224
0.002 0.003 0.002
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.262 -0.457 0.389

-0.457 -0.111 -0.250
0.389 -0.250 -0.224
0.002 -0.003 0.002
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.262 -0.457 -0.389
-0.457 -0.111 0.250
-0.389 0.250 -0.224
0.002 -0.003 -0.002
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.262 0.457 -0.389
0.457 -0.111 -0.250
-0.389 -0.250 -0.224
0.002 0.003 -0.002
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.022 0.234 -0.051
0.234 0.160 -0.071
-0.051 -0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.022 -0.234 -0.051
-0.234 0.160 0.071
-0.051 0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.022 -0.234 0.051
-0.234 0.160 -0.071
0.051 -0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.022 0.234 0.051
0.234 0.160 0.071
0.051 0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.282 0.433 0.042
0.433 -0.062 0.017
0.042 0.017 -0.242
0.006 0.002 0.001
0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 64 H
1.282 -0.433 0.042
-0.433 -0.062 -0.017
0.042 -0.017 -0.242
0.006 -0.002 0.001

-0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 65 H
1.282 -0.433 -0.042
-0.433 -0.062 0.017
-0.042 0.017 -0.242
0.006 -0.002 -0.001
-0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 66 H
1.282 0.433 -0.042
0.433 -0.062 -0.017
-0.042 -0.017 -0.242
0.006 0.002 -0.001
0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 67 H
0.124 0.201 0.098
0.201 0.018 0.074
0.098 0.074 -0.100
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.124 -0.201 0.098
-0.201 0.018 -0.074
0.098 -0.074 -0.100
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.124 -0.201 -0.098
-0.201 0.018 0.074
-0.098 0.074 -0.100
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.124 0.201 -0.098
0.201 0.018 -0.074
-0.098 -0.074 -0.100
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.039 0.173 0.008
0.173 0.044 0.014
0.008 0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.039 -0.173 0.008
-0.173 0.044 -0.014
0.008 -0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.039 -0.173 -0.008
-0.173 0.044 0.014
-0.008 0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.039 0.173 -0.008
0.173 0.044 -0.014
-0.008 -0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-219.798 -16.527 0.247
-16.527 -304.533 -32.628
0.247 -32.628 -81.387
261.916 -3.867 -0.977
-3.867 258.311 4.277
-0.977 4.277 222.786

orbtensor 2 C
-219.798 16.527 0.247
16.527 -304.533 32.628
0.247 32.628 -81.387
261.916 3.867 -0.977
3.867 258.311 -4.277
-0.977 -4.277 222.786

orbtensor 3 C
-219.798 16.527 -0.247
16.527 -304.533 -32.628
-0.247 -32.628 -81.387
261.916 3.867 0.977
3.867 258.310 4.277
0.977 4.277 222.786

orbtensor 4 C
-219.798 -16.527 -0.247
-16.527 -304.533 32.628
-0.247 32.628 -81.387
261.916 -3.867 0.977
-3.867 258.310 -4.277
0.977 -4.277 222.786

orbtensor 5 C
-277.637 -8.681 1.112
-8.681 -296.230 -21.902
1.112 -21.902 -106.798
270.796 2.396 -0.261
2.396 265.805 3.262
-0.261 3.262 228.473

orbtensor 6 C
-277.637 8.681 1.112
8.681 -296.230 21.902
1.112 21.902 -106.798
270.796 -2.396 -0.261
-2.396 265.805 -3.262
-0.261 -3.262 228.473

orbtensor 7 C
-277.637 8.681 -1.112
8.681 -296.230 -21.902

-1.112 -21.902 -106.798
270.796 -2.396 0.261
-2.396 265.805 3.262
0.261 3.262 228.473

orbtensor 8 C
-277.637 -8.681 -1.112
-8.681 -296.230 21.902
-1.112 21.902 -106.798
270.795 2.396 0.261
2.396 265.805 -3.262
0.261 -3.262 228.472

orbtensor 9 C
-249.491 -12.396 9.928
-12.396 -252.178 -11.080
9.928 -11.080 -66.308
262.720 0.698 -0.426
0.698 262.961 0.841
-0.426 0.841 217.221

orbtensor 10 C
-249.491 12.396 9.928
12.396 -252.178 11.080
9.928 11.080 -66.308
262.720 -0.698 -0.426
-0.698 262.961 -0.841
-0.426 -0.841 217.221

orbtensor 11 C
-249.491 12.396 -9.928
12.396 -252.177 -11.080
-9.928 -11.080 -66.308
262.720 -0.698 0.426
-0.698 262.961 0.841
0.426 0.841 217.221

orbtensor 12 C
-249.491 -12.396 -9.928
-12.396 -252.178 11.080
-9.928 11.080 -66.309
262.720 0.698 0.426
0.698 262.961 -0.841
0.426 -0.841 217.221

orbtensor 13 C
-287.722 -4.323 23.246
-4.323 -284.314 -1.604
23.246 -1.604 -96.264
266.346 2.106 -1.575
2.106 270.495 0.787
-1.575 0.787 228.491

orbtensor 14 C
-287.722 4.323 23.246
4.323 -284.314 1.604
23.246 1.604 -96.264
266.346 -2.106 -1.575
-2.106 270.495 -0.787
-1.575 -0.787 228.490

orbtensor 15 C
-287.722 4.323 -23.246
4.323 -284.314 -1.604
-23.246 -1.604 -96.264
266.346 -2.106 1.575
-2.106 270.495 0.787

1.575 0.787 228.491
orbtensor 16 C
-287.722 -4.323 -23.246
-4.323 -284.314 1.604
-23.246 1.604 -96.264
266.346 2.106 1.575
2.106 270.495 -0.787
1.575 -0.787 228.490

orbtensor 17 C
-220.425 -107.042 -56.328
-107.042 -218.711 58.919
-56.328 58.919 -212.040
253.905 14.332 9.928
14.332 253.937 -9.939
9.928 -9.939 249.814

orbtensor 18 C
-220.425 107.042 -56.328
107.042 -218.711 -58.919
-56.328 -58.919 -212.039
253.905 -14.332 9.928
-14.332 253.937 9.939
9.928 9.939 249.814

orbtensor 19 C
-220.425 107.042 56.328
107.042 -218.711 58.919
56.328 58.919 -212.039
253.905 -14.332 -9.928
-14.332 253.937 -9.939
-9.928 -9.939 249.814

orbtensor 20 C
-220.425 -107.042 56.328
-107.042 -218.711 -58.919
56.328 -58.919 -212.039
253.905 14.332 -9.928
14.332 253.937 9.939
-9.928 9.939 249.814

orbtensor 23 C
-199.906 69.053 90.890
69.053 -165.240 49.179
90.890 49.179 -256.951
246.835 -14.813 -6.186
-14.813 250.029 -13.239
-6.186 -13.239 249.087

orbtensor 24 C
-199.906 -69.053 90.890
-69.053 -165.240 -49.179
90.890 -49.179 -256.951
246.835 14.813 -6.186
14.813 250.029 13.239
-6.186 13.239 249.087

orbtensor 25 C
-298.442 -13.808 34.429
-13.808 -218.228 5.976
34.429 5.976 -82.159
259.034 -4.004 -3.491
-4.004 261.073 1.044
-3.491 1.044 222.064

orbtensor 26 C


```
-298.442  13.808  34.428
13.808 -218.228  -5.976
34.428  -5.976 -82.159
259.034   4.004  -3.491
4.004  261.073  -1.044
-3.491  -1.044  222.063
```

```
orbtensor 27 C
-298.442  13.808  -34.428
13.808 -218.228   5.976
-34.428   5.976 -82.159
259.034   4.004   3.491
4.004  261.073   1.044
3.491   1.044  222.064
```

```
orbtensor 28 C
-298.442  -13.808  -34.429
-13.808 -218.228  -5.976
-34.429  -5.976 -82.159
259.034  -4.004   3.491
-4.004  261.073  -1.044
3.491  -1.044  222.063
```

```
orbtensor 29 C
-164.718  -67.087  -50.667
-67.087 -194.781   89.679
-50.667   89.679 -257.645
249.703   14.878   13.275
14.878  246.374  -6.421
13.275  -6.421  248.699
```

```
orbtensor 30 C
-164.718   67.087  -50.667
67.087 -194.781  -89.679
-50.667  -89.679 -257.645
249.703  -14.878   13.275
-14.878  246.374   6.421
13.275   6.421  248.699
```

```
orbtensor 31 C
-164.718   67.087   50.667
67.087 -194.781   89.679
50.667   89.679 -257.645
249.703  -14.878  -13.275
-14.878  246.374  -6.421
-13.275  -6.421  248.699
```

```
orbtensor 32 C
-164.718  -67.087   50.667
-67.087 -194.781  -89.679
50.667  -89.679 -257.645
249.703   14.878  -13.275
14.878  246.374   6.421
-13.275   6.421  248.699
```

```
orbtensor 33 C
-153.672  -69.730  -47.690
-69.730 -193.105   99.196
-47.690   99.196 -227.627
246.002   15.537   10.651
15.537  243.801  -9.560
10.651  -9.560  245.187
```

```
orbtensor 34 C
-153.671   69.730  -47.690
69.730 -193.105  -99.195
-47.690  -99.195 -227.627
```

246.002 -15.537 10.651
-15.537 243.801 9.560
10.651 9.560 245.187

orbtensor 35 C
-153.672 69.730 47.690
69.730 -193.105 99.196
47.690 99.196 -227.627
246.002 -15.537 -10.651
-15.537 243.801 -9.560
-10.651 -9.560 245.187

orbtensor 36 C
-153.672 -69.730 47.690
-69.730 -193.105 -99.195
47.690 -99.195 -227.627
246.002 15.537 -10.651
15.537 243.801 9.560
-10.651 9.560 245.187

orbtensor 37 C
-196.533 -72.009 -98.674
-72.009 -153.027 45.511
-98.674 45.511 -225.023
244.261 15.417 9.376
15.417 246.022 -10.752
9.376 -10.752 245.480

orbtensor 38 C
-196.532 72.009 -98.674
72.009 -153.027 -45.511
-98.674 -45.511 -225.023
244.261 -15.417 9.376
-15.417 246.022 10.752
9.376 10.752 245.480

orbtensor 39 C
-196.533 72.009 98.674
72.009 -153.027 45.511
98.674 45.511 -225.023
244.261 -15.417 -9.376
-15.417 246.022 -10.752
-9.376 -10.752 245.480

orbtensor 40 C
-196.532 -72.009 98.674
-72.009 -153.027 -45.511
98.674 -45.511 -225.023
244.261 15.417 -9.376
15.417 246.022 10.752
-9.376 10.752 245.480

orbtensor 41 C
-204.564 -113.874 -52.184
-113.874 -205.269 55.381
-52.184 55.381 -176.283
245.765 12.118 10.812
12.118 245.491 -10.918
10.812 -10.918 249.845

orbtensor 42 C
-204.564 113.874 -52.184
113.874 -205.269 -55.381
-52.184 -55.381 -176.283
245.765 -12.118 10.812
-12.118 245.491 10.918
10.812 10.918 249.845

orbtensor 43 C
-204.564 113.874 52.184
113.874 -205.269 55.381
52.184 55.381 -176.283
245.765 -12.118 -10.812
-12.118 245.491 -10.918
-10.812 -10.918 249.845

orbtensor 44 C
-204.564 -113.874 52.184
-113.874 -205.269 -55.381
52.184 -55.381 -176.283
245.765 12.118 -10.812
12.118 245.491 10.918
-10.812 10.918 249.845

orbtensor 47 H
-3.904 -8.144 -1.426
-8.144 -14.349 -1.398
-1.426 -1.398 -6.636
35.327 4.785 -0.718
4.785 35.620 2.424
-0.718 2.424 18.611

orbtensor 48 H
-3.904 8.144 -1.426
8.144 -14.349 1.398
-1.426 1.398 -6.636
35.327 -4.785 -0.718
-4.785 35.620 -2.424
-0.718 -2.424 18.611

orbtensor 49 H
-3.904 8.144 1.426
8.144 -14.349 -1.398
1.426 -1.398 -6.636
35.327 -4.785 0.718
-4.785 35.620 2.424
0.718 2.424 18.611

orbtensor 50 H
-3.904 -8.144 1.426
-8.144 -14.349 1.398
1.426 1.398 -6.636
35.327 4.785 0.718
4.785 35.620 -2.424
0.718 -2.424 18.610

orbtensor 51 H
-8.946 -1.757 -10.027
-1.757 -2.727 -2.562
-10.027 -2.562 -14.002
32.448 4.565 5.548
4.565 27.218 -3.800
5.548 -3.800 33.438

orbtensor 52 H
-8.946 1.757 -10.027
1.757 -2.727 2.562
-10.027 2.562 -14.002
32.448 -4.565 5.548
-4.565 27.218 3.800
5.548 3.800 33.438

orbtensor 53 H
-8.946 1.757 10.027

1.757	-2.727	-2.562
10.027	-2.562	-14.002
32.448	-4.565	-5.548
-4.565	27.218	-3.800
-5.548	-3.800	33.438

orbtensor 54 H

-8.946	-1.757	10.027
-1.757	-2.727	2.562
10.027	2.562	-14.002
32.448	4.565	-5.548
4.565	27.218	3.800
-5.548	3.800	33.438

orbtensor 55 H

-2.506	-1.223	2.043
-1.223	-8.569	9.911
2.043	9.911	-14.864
27.164	4.054	4.168
4.054	32.304	-5.470
4.168	-5.470	34.066

orbtensor 56 H

-2.506	1.223	2.043
1.223	-8.569	-9.911
2.043	-9.911	-14.864
27.164	-4.054	4.168
-4.054	32.304	5.470
4.168	5.470	34.066

orbtensor 57 H

-2.506	1.223	-2.043
1.223	-8.569	9.911
-2.043	9.911	-14.864
27.164	-4.054	-4.168
-4.054	32.304	-5.470
-4.168	-5.470	34.066

orbtensor 58 H

-2.506	-1.223	-2.043
-1.223	-8.569	-9.911
-2.043	-9.911	-14.864
27.164	4.054	-4.168
4.054	32.304	5.470
-4.168	5.470	34.065

orbtensor 59 H

-1.987	-1.121	0.424
-1.121	-9.304	7.715
0.424	7.715	-12.819
27.008	3.716	0.808
3.716	32.777	-9.059
0.808	-9.059	33.948

orbtensor 60 H

-1.987	1.121	0.424
1.121	-9.304	-7.715
0.424	-7.715	-12.819
27.008	-3.716	0.808
-3.716	32.777	9.059
0.808	9.059	33.948

orbtensor 61 H

-1.987	1.121	-0.424
1.121	-9.304	7.715
-0.424	7.715	-12.819
27.008	-3.716	-0.808

-3.716 32.777 -9.059
-0.808 -9.059 33.948

orbtensor 62 H
-1.987 -1.121 -0.424
-1.121 -9.304 -7.715
-0.424 -7.715 -12.819
27.008 3.716 -0.808
3.716 32.777 9.059
-0.808 9.059 33.948

orbtensor 63 H
-14.105 -7.983 1.406
-7.983 -3.770 1.604
1.406 1.604 -6.565
36.312 4.833 -1.935
4.833 35.277 0.704
-1.935 0.704 18.411

orbtensor 64 H
-14.105 7.983 1.406
7.983 -3.770 -1.604
1.406 -1.604 -6.565
36.312 -4.833 -1.935
-4.833 35.277 -0.704
-1.935 -0.704 18.410

orbtensor 65 H
-14.105 7.983 -1.406
7.983 -3.770 1.604
-1.406 1.604 -6.565
36.312 -4.833 1.935
-4.833 35.277 0.704
1.935 0.704 18.411

orbtensor 66 H
-14.105 -7.983 -1.406
-7.983 -3.770 -1.604
-1.406 -1.604 -6.565
36.312 4.833 1.935
4.833 35.277 -0.704
1.935 -0.704 18.410

orbtensor 67 H
-9.687 -1.440 -7.764
-1.440 -2.083 -0.777
-7.764 -0.777 -12.439
33.174 3.940 9.038
3.940 27.077 -0.565
9.038 -0.565 33.619

orbtensor 68 H
-9.687 1.440 -7.764
1.440 -2.083 0.777
-7.764 0.777 -12.439
33.174 -3.940 9.038
-3.940 27.077 0.565
9.038 0.565 33.619

orbtensor 69 H
-9.687 1.440 7.764
1.440 -2.083 -0.777
7.764 -0.777 -12.438
33.174 -3.940 -9.038
-3.940 27.077 -0.565
-9.038 -0.565 33.619

```

orbtensor 70 H
-9.687  -1.440   7.764
-1.440  -2.083   0.777
7.764   0.777  -12.439
33.174  3.940  -9.038
3.940   27.077  0.565
-9.038   0.565  33.619

```

```

orbtensor 71 H
-10.488  -8.892   0.319
-8.892 -10.747   0.152
0.319   0.152  -3.201
33.752   9.672   1.584
9.672  33.908  -2.015
1.584  -2.015  26.546

```

```

orbtensor 72 H
-10.488   8.892   0.319
8.892 -10.747  -0.152
0.319  -0.152  -3.201
33.752  -9.672   1.584
-9.672  33.908   2.015
1.584   2.015  26.546

```

```

orbtensor 73 H
-10.488   8.892  -0.319
8.892 -10.747   0.152
-0.319   0.152  -3.201
33.752  -9.672  -1.584
-9.672  33.908  -2.015
-1.584  -2.015  26.546

```

```

orbtensor 74 H
-10.488  -8.892  -0.319
-8.892 -10.747  -0.152
-0.319  -0.152  -3.201
33.752   9.672  -1.584
9.672  33.908   2.015
-1.584   2.015  26.546

```

```

gtensor (ppt)
-0.175   0.000   0.000
0.000  -0.177   0.000
0.000   0.000  -0.167
13.608   0.000   0.000
0.000  15.405   0.000
0.000   0.000   4.418

```

```

zfstensor (cm-1)
-0.335571  0.000004  0.000001
0.000004  -0.437059  -0.000068
0.000001  -0.000068  1.385620

```

```

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9737	45.76500	-1183.65137	-3.08262	-1186.73400	-1140.96900
2	C	0.9737	45.76500	-1183.65137	-3.08244	-1186.73381	-1140.96881
3	C	0.9737	45.76467	-1183.65137	-3.08263	-1186.73400	-1140.96934
4	C	0.9737	45.76467	-1183.65137	-3.08243	-1186.73380	-1140.96914
5	C	0.9183	28.13633	-1116.38464	-12.23946	-1128.62410	-1100.48776

6	C	0.9183	28.13633	-1116.38464	-12.23901	-1128.62365	-1100.48732
7	C	0.9183	28.13633	-1116.38464	-12.23954	-1128.62418	-1100.48785
8	C	0.9183	28.13567	-1116.38464	-12.23893	-1128.62357	-1100.48791
9	C	0.2787	58.30833	-338.76499	1.65530	-337.10969	-278.80136
10	C	0.2787	58.30833	-338.76499	1.65548	-337.10952	-278.80118
11	C	0.2787	58.30867	-338.76499	1.65524	-337.10976	-278.80109
12	C	0.2787	58.30800	-338.76499	1.65553	-337.10946	-278.80146
13	C	0.4977	32.34400	-604.99538	-11.23289	-616.22827	-583.88427
14	C	0.4977	32.34367	-604.99538	-11.23290	-616.22828	-583.88462
15	C	0.4977	32.34400	-604.99538	-11.23298	-616.22835	-583.88435
16	C	0.4977	32.34367	-604.99538	-11.23283	-616.22821	-583.88454
17	C	-0.1840	35.49333	223.68215	-1.95787	221.72428	257.21761
18	C	-0.1840	35.49367	223.68215	-1.95787	221.72428	257.21794
19	C	-0.1840	35.49367	223.68215	-1.95790	221.72425	257.21792
20	C	-0.1840	35.49367	223.68215	-1.95785	221.72430	257.21797
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1957	41.28467	-237.86489	-1.59537	-239.46026	-198.17560
24	C	0.1957	41.28467	-237.86489	-1.59539	-239.46028	-198.17561
25	C	1.0860	47.78067	-1320.21095	-2.86667	-1323.07761	-1275.29695
26	C	1.0860	47.78033	-1320.21095	-2.86664	-1323.07758	-1275.29725
27	C	1.0860	47.78067	-1320.21095	-2.86668	-1323.07762	-1275.29696
28	C	1.0860	47.78033	-1320.21095	-2.86663	-1323.07757	-1275.29724
29	C	0.1890	42.54400	-229.76047	-1.16311	-230.92358	-188.37958
30	C	0.1890	42.54400	-229.76047	-1.16303	-230.92350	-188.37950
31	C	0.1890	42.54400	-229.76047	-1.16312	-230.92359	-188.37959
32	C	0.1890	42.54400	-229.76047	-1.16302	-230.92349	-188.37949
33	C	0.0003	53.52867	-0.40522	-0.69986	-1.10508	52.42358
34	C	0.0003	53.52900	-0.40522	-0.69990	-1.10512	52.42388
35	C	0.0003	53.52867	-0.40522	-0.69987	-1.10509	52.42357
36	C	0.0003	53.52867	-0.40522	-0.69989	-1.10512	52.42355
A Average		0.7080	30.24000	-860.69001	-11.73607	-872.42608	-842.18608
B Average		1.0298	46.77267	-1251.93116	-2.97459	-1254.90575	-1208.13308
M Average		0.2787	58.30833	-338.76499	1.65539	-337.10961	-278.80127

=====

FeL5-saddled-HS-STO-PBE0-No-ZFS

Temperature: 303

Spin: 2.5

atensor 1 C

0.687 0.061 0.014
0.061 1.476 0.115
0.014 0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C

0.687 -0.061 0.014
-0.061 1.476 -0.115
0.014 -0.115 0.766
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C

0.687 -0.061 -0.014
-0.061 1.476 0.115
-0.014 0.115 0.766
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C

0.687 0.061 -0.014

0.061 1.476 -0.115
-0.014 -0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.790 0.802 0.105
0.802 1.951 0.315
0.105 0.315 0.010
-0.003 0.005 0.000
0.007 0.005 0.001
0.000 0.001 0.002

atensor 6 C
0.790 -0.802 0.105
-0.802 1.951 -0.315
0.105 -0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 7 C
0.790 -0.802 -0.105
-0.802 1.951 0.315
-0.105 0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 0.001
0.000 0.001 0.002

atensor 8 C
0.790 0.802 -0.105
0.802 1.951 -0.315
-0.105 -0.315 0.010
-0.003 0.005 0.000
0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 9 C
0.207 0.595 0.154
0.595 0.224 0.142
0.154 0.142 0.408
-0.001 -0.002 0.001
-0.004 -0.002 0.001
0.001 0.000 0.000

atensor 10 C
0.207 -0.595 0.154
-0.595 0.224 -0.142
0.154 -0.142 0.408
-0.001 0.002 0.001
0.004 -0.002 -0.001
0.001 0.000 0.000

atensor 11 C
0.207 -0.595 -0.154
-0.595 0.224 0.142
-0.154 0.142 0.408
-0.001 0.002 -0.001
0.004 -0.002 0.001
-0.001 0.000 0.000

atensor 12 C
0.207 0.595 -0.154
0.595 0.224 -0.142
-0.154 -0.142 0.408
-0.001 -0.002 -0.001

-0.004 -0.002 -0.001
-0.001 0.000 0.000

atensor 13 C
1.511 0.799 0.149
0.799 0.400 0.042
0.149 0.042 -0.420
0.003 0.006 0.001
0.005 -0.002 0.000
0.001 -0.002 0.001

atensor 14 C
1.511 -0.799 0.149
-0.799 0.400 -0.042
0.149 -0.042 -0.420
0.003 -0.006 0.001
-0.005 -0.002 0.000
0.001 0.002 0.001

atensor 15 C
1.511 -0.799 -0.149
-0.799 0.400 0.042
-0.149 0.042 -0.420
0.003 -0.006 -0.001
-0.005 -0.002 0.000
-0.001 -0.002 0.001

atensor 16 C
1.511 0.799 -0.149
0.799 0.400 -0.042
-0.149 -0.042 -0.420
0.003 0.006 -0.001
0.005 -0.002 0.000
-0.001 0.002 0.001

atensor 17 C
-0.112 0.242 0.049
0.242 -0.105 0.014
0.049 0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.112 -0.242 0.049
-0.242 -0.105 -0.014
0.049 -0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.112 -0.242 -0.049
-0.242 -0.105 0.014
-0.049 0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.112 0.242 -0.049
0.242 -0.105 -0.014
-0.049 -0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.199 -0.132 0.028
-0.132 0.311 -0.017
0.028 -0.017 0.076
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.199 0.132 0.028
0.132 0.311 0.017
0.028 0.017 0.076
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.639 0.086 -0.011
0.086 0.799 0.023
-0.011 0.023 0.831
0.002 -0.001 0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 26 C
1.639 -0.086 -0.011
-0.086 0.799 -0.023
-0.011 -0.023 0.831
0.002 0.001 0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 27 C
1.639 -0.086 0.011
-0.086 0.799 0.023
0.011 0.023 0.831
0.002 0.001 -0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 28 C
1.639 0.086 0.011
0.086 0.799 -0.023
0.011 -0.023 0.831
0.002 -0.001 -0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 29 C
0.282 0.110 0.044
0.110 0.190 0.053
0.044 0.053 0.095
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.282 -0.110 0.044
-0.110 0.190 -0.053
0.044 -0.053 0.095
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.282 -0.110 -0.044
-0.110 0.190 0.053

-0.044 0.053 0.095
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.282 0.110 -0.044
0.110 0.190 -0.053
-0.044 -0.053 0.095
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.013 0.093 -0.001
0.093 0.041 -0.019
-0.001 -0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.013 -0.093 -0.001
-0.093 0.041 0.019
-0.001 0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.013 -0.093 0.001
-0.093 0.041 -0.019
0.001 -0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.013 0.093 0.001
0.093 0.041 0.019
0.001 0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.033 0.085 0.032
0.085 0.010 0.012
0.032 0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.033 -0.085 0.032
-0.085 0.011 -0.012
0.032 -0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.033 -0.085 -0.032
-0.085 0.011 0.012
-0.032 0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000

0.000 0.000 0.000

atensor 40 C
0.033 0.085 -0.032
0.085 0.011 -0.012
-0.032 -0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.043 0.045 -0.010
0.045 0.045 0.020
-0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.043 -0.045 -0.010
-0.045 0.045 -0.020
-0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.043 -0.045 0.010
-0.045 0.045 0.020
0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.043 0.045 0.010
0.045 0.045 -0.020
0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.176 0.408 0.068
0.408 1.085 0.236
0.068 0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 0.002
0.000 0.000 -0.001

atensor 48 H
-0.176 -0.408 0.068
-0.408 1.085 -0.236
0.068 -0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 49 H
-0.176 -0.408 -0.068
-0.408 1.085 0.236
-0.068 0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 0.002
0.000 0.000 -0.001

atensor 50 H

-0.176 0.408 -0.068
0.408 1.085 -0.236
-0.068 -0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 51 H
-0.112 0.622 -0.191
0.622 0.452 -0.314
-0.191 -0.314 -0.411
-0.001 0.005 -0.001
0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 52 H
-0.112 -0.622 -0.191
-0.622 0.452 0.314
-0.191 0.314 -0.411
-0.001 -0.005 -0.001
-0.005 0.004 0.002
0.000 0.001 -0.001

atensor 53 H
-0.112 -0.622 0.191
-0.622 0.452 -0.314
0.191 -0.314 -0.411
-0.001 -0.005 0.001
-0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 54 H
-0.112 0.622 0.191
0.622 0.452 0.314
0.191 0.314 -0.411
-0.001 0.005 0.001
0.005 0.004 0.002
0.000 0.001 -0.001

atensor 55 H
0.262 0.457 0.389
0.457 -0.111 0.250
0.389 0.250 -0.224
0.002 0.003 0.002
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.262 -0.457 0.389
-0.457 -0.111 -0.250
0.389 -0.250 -0.224
0.002 -0.003 0.002
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.262 -0.457 -0.389
-0.457 -0.111 0.250
-0.389 0.250 -0.224
0.002 -0.003 -0.002
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.262 0.457 -0.389
0.457 -0.111 -0.250
-0.389 -0.250 -0.224

0.002 0.003 -0.002
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.022 0.234 -0.051
0.234 0.160 -0.071
-0.051 -0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.022 -0.234 -0.051
-0.234 0.160 0.071
-0.051 0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.022 -0.234 0.051
-0.234 0.160 -0.071
0.051 -0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.022 0.234 0.051
0.234 0.160 0.071
0.051 0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.282 0.433 0.042
0.433 -0.062 0.017
0.042 0.017 -0.242
0.006 0.002 0.001
0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 64 H
1.282 -0.433 0.042
-0.433 -0.062 -0.017
0.042 -0.017 -0.242
0.006 -0.002 0.001
-0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 65 H
1.282 -0.433 -0.042
-0.433 -0.062 0.017
-0.042 0.017 -0.242
0.006 -0.002 -0.001
-0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 66 H
1.282 0.433 -0.042
0.433 -0.062 -0.017
-0.042 -0.017 -0.242
0.006 0.002 -0.001
0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 67 H
0.124 0.201 0.098
0.201 0.018 0.074
0.098 0.074 -0.100
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.124 -0.201 0.098
-0.201 0.018 -0.074
0.098 -0.074 -0.100
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.124 -0.201 -0.098
-0.201 0.018 0.074
-0.098 0.074 -0.100
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.124 0.201 -0.098
0.201 0.018 -0.074
-0.098 -0.074 -0.100
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.039 0.173 0.008
0.173 0.044 0.014
0.008 0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.039 -0.173 0.008
-0.173 0.044 -0.014
0.008 -0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.039 -0.173 -0.008
-0.173 0.044 0.014
-0.008 0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.039 0.173 -0.008
0.173 0.044 -0.014
-0.008 -0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-219.798 -16.527 0.247

-16.527 -304.533 -32.628
0.247 -32.628 -81.387
261.916 -3.867 -0.977
-3.867 258.311 4.277
-0.977 4.277 222.786

orbtensor 2 C
-219.798 16.527 0.247
16.527 -304.533 32.628
0.247 32.628 -81.387
261.916 3.867 -0.977
3.867 258.311 -4.277
-0.977 -4.277 222.786

orbtensor 3 C
-219.798 16.527 -0.247
16.527 -304.533 -32.628
-0.247 -32.628 -81.387
261.916 3.867 0.977
3.867 258.310 4.277
0.977 4.277 222.786

orbtensor 4 C
-219.798 -16.527 -0.247
-16.527 -304.533 32.628
-0.247 32.628 -81.387
261.916 -3.867 0.977
-3.867 258.310 -4.277
0.977 -4.277 222.786

orbtensor 5 C
-277.637 -8.681 1.112
-8.681 -296.230 -21.902
1.112 -21.902 -106.798
270.796 2.396 -0.261
2.396 265.805 3.262
-0.261 3.262 228.473

orbtensor 6 C
-277.637 8.681 1.112
8.681 -296.230 21.902
1.112 21.902 -106.798
270.796 -2.396 -0.261
-2.396 265.805 -3.262
-0.261 -3.262 228.473

orbtensor 7 C
-277.637 8.681 -1.112
8.681 -296.230 -21.902
-1.112 -21.902 -106.798
270.796 -2.396 0.261
-2.396 265.805 3.262
0.261 3.262 228.473

orbtensor 8 C
-277.637 -8.681 -1.112
-8.681 -296.230 21.902
-1.112 21.902 -106.798
270.795 2.396 0.261
2.396 265.805 -3.262
0.261 -3.262 228.472

orbtensor 9 C
-249.491 -12.396 9.928
-12.396 -252.178 -11.080
9.928 -11.080 -66.308
262.720 0.698 -0.426

0.698 262.961 0.841
-0.426 0.841 217.221

orbtensor 10 C
-249.491 12.396 9.928
12.396 -252.178 11.080
9.928 11.080 -66.308
262.720 -0.698 -0.426
-0.698 262.961 -0.841
-0.426 -0.841 217.221

orbtensor 11 C
-249.491 12.396 -9.928
12.396 -252.177 -11.080
-9.928 -11.080 -66.308
262.720 -0.698 0.426
-0.698 262.961 0.841
0.426 0.841 217.221

orbtensor 12 C
-249.491 -12.396 -9.928
-12.396 -252.178 11.080
-9.928 11.080 -66.309
262.720 0.698 0.426
0.698 262.961 -0.841
0.426 -0.841 217.221

orbtensor 13 C
-287.722 -4.323 23.246
-4.323 -284.314 -1.604
23.246 -1.604 -96.264
266.346 2.106 -1.575
2.106 270.495 0.787
-1.575 0.787 228.491

orbtensor 14 C
-287.722 4.323 23.246
4.323 -284.314 1.604
23.246 1.604 -96.264
266.346 -2.106 -1.575
-2.106 270.495 -0.787
-1.575 -0.787 228.490

orbtensor 15 C
-287.722 4.323 -23.246
4.323 -284.314 -1.604
-23.246 -1.604 -96.264
266.346 -2.106 1.575
-2.106 270.495 0.787
1.575 0.787 228.491

orbtensor 16 C
-287.722 -4.323 -23.246
-4.323 -284.314 1.604
-23.246 1.604 -96.264
266.346 2.106 1.575
2.106 270.495 -0.787
1.575 -0.787 228.490

orbtensor 17 C
-220.425 -107.042 -56.328
-107.042 -218.711 58.919
-56.328 58.919 -212.040
253.905 14.332 9.928
14.332 253.937 -9.939
9.928 -9.939 249.814

orbtensor 18 C
-220.425 107.042 -56.328
107.042 -218.711 -58.919
-56.328 -58.919 -212.039
253.905 -14.332 9.928
-14.332 253.937 9.939
9.928 9.939 249.814

orbtensor 19 C
-220.425 107.042 56.328
107.042 -218.711 58.919
56.328 58.919 -212.039
253.905 -14.332 -9.928
-14.332 253.937 -9.939
-9.928 -9.939 249.814

orbtensor 20 C
-220.425 -107.042 56.328
-107.042 -218.711 -58.919
56.328 -58.919 -212.039
253.905 14.332 -9.928
14.332 253.937 9.939
-9.928 9.939 249.814

orbtensor 23 C
-199.906 69.053 90.890
69.053 -165.240 49.179
90.890 49.179 -256.951
246.835 -14.813 -6.186
-14.813 250.029 -13.239
-6.186 -13.239 249.087

orbtensor 24 C
-199.906 -69.053 90.890
-69.053 -165.240 -49.179
90.890 -49.179 -256.951
246.835 14.813 -6.186
14.813 250.029 13.239
-6.186 13.239 249.087

orbtensor 25 C
-298.442 -13.808 34.429
-13.808 -218.228 5.976
34.429 5.976 -82.159
259.034 -4.004 -3.491
-4.004 261.073 1.044
-3.491 1.044 222.064

orbtensor 26 C
-298.442 13.808 34.428
13.808 -218.228 -5.976
34.428 -5.976 -82.159
259.034 4.004 -3.491
4.004 261.073 -1.044
-3.491 -1.044 222.063

orbtensor 27 C
-298.442 13.808 -34.428
13.808 -218.228 5.976
-34.428 5.976 -82.159
259.034 4.004 3.491
4.004 261.073 1.044
3.491 1.044 222.064

orbtensor 28 C
-298.442 -13.808 -34.429
-13.808 -218.228 -5.976

-34.429	-5.976	-82.159
259.034	-4.004	3.491
-4.004	261.073	-1.044
3.491	-1.044	222.063

orbtensor 29 C

-164.718	-67.087	-50.667
-67.087	-194.781	89.679
-50.667	89.679	-257.645
249.703	14.878	13.275
14.878	246.374	-6.421
13.275	-6.421	248.699

orbtensor 30 C

-164.718	67.087	-50.667
67.087	-194.781	-89.679
-50.667	-89.679	-257.645
249.703	-14.878	13.275
-14.878	246.374	6.421
13.275	6.421	248.699

orbtensor 31 C

-164.718	67.087	50.667
67.087	-194.781	89.679
50.667	89.679	-257.645
249.703	-14.878	-13.275
-14.878	246.374	-6.421
-13.275	-6.421	248.699

orbtensor 32 C

-164.718	-67.087	50.667
-67.087	-194.781	-89.679
50.667	-89.679	-257.645
249.703	14.878	-13.275
14.878	246.374	6.421
-13.275	6.421	248.699

orbtensor 33 C

-153.672	-69.730	-47.690
-69.730	-193.105	99.196
-47.690	99.196	-227.627
246.002	15.537	10.651
15.537	243.801	-9.560
10.651	-9.560	245.187

orbtensor 34 C

-153.671	69.730	-47.690
69.730	-193.105	-99.195
-47.690	-99.195	-227.627
246.002	-15.537	10.651
-15.537	243.801	9.560
10.651	9.560	245.187

orbtensor 35 C

-153.672	69.730	47.690
69.730	-193.105	99.196
47.690	99.196	-227.627
246.002	-15.537	-10.651
-15.537	243.801	-9.560
-10.651	-9.560	245.187

orbtensor 36 C

-153.672	-69.730	47.690
-69.730	-193.105	-99.195
47.690	-99.195	-227.627
246.002	15.537	-10.651
15.537	243.801	9.560

-10.651 9.560 245.187

orbtensor 37 C

-196.533 -72.009 -98.674
-72.009 -153.027 45.511
-98.674 45.511 -225.023
244.261 15.417 9.376
15.417 246.022 -10.752
9.376 -10.752 245.480

orbtensor 38 C

-196.532 72.009 -98.674
72.009 -153.027 -45.511
-98.674 -45.511 -225.023
244.261 -15.417 9.376
-15.417 246.022 10.752
9.376 10.752 245.480

orbtensor 39 C

-196.533 72.009 98.674
72.009 -153.027 45.511
98.674 45.511 -225.023
244.261 -15.417 -9.376
-15.417 246.022 -10.752
-9.376 -10.752 245.480

orbtensor 40 C

-196.532 -72.009 98.674
-72.009 -153.027 -45.511
98.674 -45.511 -225.023
244.261 15.417 -9.376
15.417 246.022 10.752
-9.376 10.752 245.480

orbtensor 41 C

-204.564 -113.874 -52.184
-113.874 -205.269 55.381
-52.184 55.381 -176.283
245.765 12.118 10.812
12.118 245.491 -10.918
10.812 -10.918 249.845

orbtensor 42 C

-204.564 113.874 -52.184
113.874 -205.269 -55.381
-52.184 -55.381 -176.283
245.765 -12.118 10.812
-12.118 245.491 10.918
10.812 10.918 249.845

orbtensor 43 C

-204.564 113.874 52.184
113.874 -205.269 55.381
52.184 55.381 -176.283
245.765 -12.118 -10.812
-12.118 245.491 -10.918
-10.812 -10.918 249.845

orbtensor 44 C

-204.564 -113.874 52.184
-113.874 -205.269 -55.381
52.184 -55.381 -176.283
245.765 12.118 -10.812
12.118 245.491 10.918
-10.812 10.918 249.845

orbtensor 47 H

-3.904	-8.144	-1.426
-8.144	-14.349	-1.398
-1.426	-1.398	-6.636
35.327	4.785	-0.718
4.785	35.620	2.424
-0.718	2.424	18.611

orbtensor 48 H

-3.904	8.144	-1.426
8.144	-14.349	1.398
-1.426	1.398	-6.636
35.327	-4.785	-0.718
-4.785	35.620	-2.424
-0.718	-2.424	18.611

orbtensor 49 H

-3.904	8.144	1.426
8.144	-14.349	-1.398
1.426	-1.398	-6.636
35.327	-4.785	0.718
-4.785	35.620	2.424
0.718	2.424	18.611

orbtensor 50 H

-3.904	-8.144	1.426
-8.144	-14.349	1.398
1.426	1.398	-6.636
35.327	4.785	0.718
4.785	35.620	-2.424
0.718	-2.424	18.610

orbtensor 51 H

-8.946	-1.757	-10.027
-1.757	-2.727	-2.562
-10.027	-2.562	-14.002
32.448	4.565	5.548
4.565	27.218	-3.800
5.548	-3.800	33.438

orbtensor 52 H

-8.946	1.757	-10.027
1.757	-2.727	2.562
-10.027	2.562	-14.002
32.448	-4.565	5.548
-4.565	27.218	3.800
5.548	3.800	33.438

orbtensor 53 H

-8.946	1.757	10.027
1.757	-2.727	-2.562
10.027	-2.562	-14.002
32.448	-4.565	-5.548
-4.565	27.218	-3.800
-5.548	-3.800	33.438

orbtensor 54 H

-8.946	-1.757	10.027
-1.757	-2.727	2.562
10.027	2.562	-14.002
32.448	4.565	-5.548
4.565	27.218	3.800
-5.548	3.800	33.438

orbtensor 55 H

-2.506	-1.223	2.043
-1.223	-8.569	9.911
2.043	9.911	-14.864

27.164	4.054	4.168
4.054	32.304	-5.470
4.168	-5.470	34.066

orbtensor 56 H

-2.506	1.223	2.043
1.223	-8.569	-9.911
2.043	-9.911	-14.864
27.164	-4.054	4.168
-4.054	32.304	5.470
4.168	5.470	34.066

orbtensor 57 H

-2.506	1.223	-2.043
1.223	-8.569	9.911
-2.043	9.911	-14.864
27.164	-4.054	-4.168
-4.054	32.304	-5.470
-4.168	-5.470	34.066

orbtensor 58 H

-2.506	-1.223	-2.043
-1.223	-8.569	-9.911
-2.043	-9.911	-14.864
27.164	4.054	-4.168
4.054	32.304	5.470
-4.168	5.470	34.065

orbtensor 59 H

-1.987	-1.121	0.424
-1.121	-9.304	7.715
0.424	7.715	-12.819
27.008	3.716	0.808
3.716	32.777	-9.059
0.808	-9.059	33.948

orbtensor 60 H

-1.987	1.121	0.424
1.121	-9.304	-7.715
0.424	-7.715	-12.819
27.008	-3.716	0.808
-3.716	32.777	9.059
0.808	9.059	33.948

orbtensor 61 H

-1.987	1.121	-0.424
1.121	-9.304	7.715
-0.424	7.715	-12.819
27.008	-3.716	-0.808
-3.716	32.777	-9.059
-0.808	-9.059	33.948

orbtensor 62 H

-1.987	-1.121	-0.424
-1.121	-9.304	-7.715
-0.424	-7.715	-12.819
27.008	3.716	-0.808
3.716	32.777	9.059
-0.808	9.059	33.948

orbtensor 63 H

-14.105	-7.983	1.406
-7.983	-3.770	1.604
1.406	1.604	-6.565
36.312	4.833	-1.935
4.833	35.277	0.704
-1.935	0.704	18.411

orbtensor 64 H
-14.105 7.983 1.406
7.983 -3.770 -1.604
1.406 -1.604 -6.565
36.312 -4.833 -1.935
-4.833 35.277 -0.704
-1.935 -0.704 18.410

orbtensor 65 H
-14.105 7.983 -1.406
7.983 -3.770 1.604
-1.406 1.604 -6.565
36.312 -4.833 1.935
-4.833 35.277 0.704
1.935 0.704 18.411

orbtensor 66 H
-14.105 -7.983 -1.406
-7.983 -3.770 -1.604
-1.406 -1.604 -6.565
36.312 4.833 1.935
4.833 35.277 -0.704
1.935 -0.704 18.410

orbtensor 67 H
-9.687 -1.440 -7.764
-1.440 -2.083 -0.777
-7.764 -0.777 -12.439
33.174 3.940 9.038
3.940 27.077 -0.565
9.038 -0.565 33.619

orbtensor 68 H
-9.687 1.440 -7.764
1.440 -2.083 0.777
-7.764 0.777 -12.439
33.174 -3.940 9.038
-3.940 27.077 0.565
9.038 0.565 33.619

orbtensor 69 H
-9.687 1.440 7.764
1.440 -2.083 -0.777
7.764 -0.777 -12.438
33.174 -3.940 -9.038
-3.940 27.077 -0.565
-9.038 -0.565 33.619

orbtensor 70 H
-9.687 -1.440 7.764
-1.440 -2.083 0.777
7.764 0.777 -12.439
33.174 3.940 -9.038
3.940 27.077 0.565
-9.038 0.565 33.619

orbtensor 71 H
-10.488 -8.892 0.319
-8.892 -10.747 0.152
0.319 0.152 -3.201
33.752 9.672 1.584
9.672 33.908 -2.015
1.584 -2.015 26.546

orbtensor 72 H
-10.488 8.892 0.319

```

8.892  -10.747  -0.152
0.319  -0.152   -3.201
33.752  -9.672   1.584
-9.672  33.908   2.015
1.584   2.015   26.546

```

```

orbtensor 73 H
-10.488   8.892   -0.319
8.892  -10.747   0.152
-0.319   0.152  -3.201
33.752  -9.672  -1.584
-9.672  33.908  -2.015
-1.584  -2.015  26.546

```

```

orbtensor 74 H
-10.488  -8.892   -0.319
-8.892  -10.747  -0.152
-0.319  -0.152  -3.201
33.752   9.672  -1.584
9.672  33.908   2.015
-1.584   2.015  26.546

```

```

gtensor (ppt)
-0.175   0.000   0.000
0.000  -0.177   0.000
0.000   0.000  -0.167
13.608   0.000   0.000
0.000  15.405   0.000
0.000   0.000   4.418

```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9737	45.76500	-1183.64558	-0.56784	-1184.21342	-1138.44842
2	C	0.9737	45.76500	-1183.64558	-0.56784	-1184.21342	-1138.44842
3	C	0.9737	45.76467	-1183.64558	-0.56784	-1184.21342	-1138.44876
4	C	0.9737	45.76467	-1183.64558	-0.56784	-1184.21342	-1138.44876
5	C	0.9183	28.13633	-1116.37918	-2.04987	-1118.42905	-1090.29271
6	C	0.9183	28.13633	-1116.37918	-2.04987	-1118.42905	-1090.29271
7	C	0.9183	28.13633	-1116.37918	-2.04987	-1118.42905	-1090.29271
8	C	0.9183	28.13567	-1116.37918	-2.04987	-1118.42905	-1090.29338
9	C	0.2787	58.30833	-338.76334	0.25949	-338.50385	-280.19551
10	C	0.2787	58.30833	-338.76334	0.25949	-338.50385	-280.19551
11	C	0.2787	58.30867	-338.76334	0.25949	-338.50385	-280.19518
12	C	0.2787	58.30800	-338.76334	0.25949	-338.50385	-280.19585
13	C	0.4977	32.34400	-604.99242	-1.65807	-606.65049	-574.30649
14	C	0.4977	32.34367	-604.99242	-1.65807	-606.65049	-574.30682
15	C	0.4977	32.34400	-604.99242	-1.65807	-606.65049	-574.30649
16	C	0.4977	32.34367	-604.99242	-1.65807	-606.65049	-574.30682
17	C	-0.1840	35.49333	223.68105	-0.30945	223.37161	258.86494
18	C	-0.1840	35.49367	223.68105	-0.30945	223.37161	258.86527
19	C	-0.1840	35.49367	223.68105	-0.30945	223.37161	258.86527
20	C	-0.1840	35.49367	223.68105	-0.30945	223.37161	258.86527
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1957	41.28467	-237.86373	-0.26318	-238.12691	-196.84225
24	C	0.1957	41.28467	-237.86373	-0.26318	-238.12691	-196.84225
25	C	1.0860	47.78067	-1320.20449	-0.36509	-1320.56957	-1272.78891
26	C	1.0860	47.78033	-1320.20449	-0.36509	-1320.56957	-1272.78924
27	C	1.0860	47.78067	-1320.20449	-0.36509	-1320.56957	-1272.78891
28	C	1.0860	47.78033	-1320.20449	-0.36509	-1320.56957	-1272.78924

29	C	0.1890	42.54400	-229.75934	-0.17408	-229.93343	-187.38943
30	C	0.1890	42.54400	-229.75934	-0.17408	-229.93343	-187.38943
31	C	0.1890	42.54400	-229.75934	-0.17408	-229.93343	-187.38943
32	C	0.1890	42.54400	-229.75934	-0.17408	-229.93343	-187.38943
33	C	0.0003	53.52867	-0.40522	-0.11326	-0.51848	53.01019
34	C	0.0003	53.52900	-0.40522	-0.11326	-0.51848	53.01052
35	C	0.0003	53.52867	-0.40522	-0.11326	-0.51848	53.01019
36	C	0.0003	53.52867	-0.40522	-0.11326	-0.51848	53.01019
A Average		0.7080	30.24000	-860.68580	-1.85397	-862.53977	-832.29977
B Average		1.0298	46.77267	-1251.92503	-0.46646	-1252.39150	-1205.61883
M Average		0.2787	58.30833	-338.76334	0.25949	-338.50385	-280.19551

=====

FeL5-saddled-HS-STO-PBE0-No-G

Temperature: 303

Spin: 2.5

atensor 1 C

0.687 0.061 0.014
0.061 1.476 0.115
0.014 0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C

0.687 -0.061 0.014
-0.061 1.476 -0.115
0.014 -0.115 0.766
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C

0.687 -0.061 -0.014
-0.061 1.476 0.115
-0.014 0.115 0.766
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C

0.687 0.061 -0.014
0.061 1.476 -0.115
-0.014 -0.115 0.766
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C

0.790 0.802 0.105
0.802 1.951 0.315
0.105 0.315 0.010
-0.003 0.005 0.000
0.007 0.005 0.001
0.000 0.001 0.002

atensor 6 C

0.790 -0.802 0.105
-0.802 1.951 -0.315
0.105 -0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 7 C

0.790 -0.802 -0.105
-0.802 1.951 0.315
-0.105 0.315 0.010
-0.003 -0.005 0.000
-0.007 0.005 0.001
0.000 0.001 0.002

atensor 8 C
0.790 0.802 -0.105
0.802 1.951 -0.315
-0.105 -0.315 0.010
-0.003 0.005 0.000
0.007 0.005 -0.001
0.000 -0.001 0.002

atensor 9 C
0.207 0.595 0.154
0.595 0.224 0.142
0.154 0.142 0.408
-0.001 -0.002 0.001
-0.004 -0.002 0.001
0.001 0.000 0.000

atensor 10 C
0.207 -0.595 0.154
-0.595 0.224 -0.142
0.154 -0.142 0.408
-0.001 0.002 0.001
0.004 -0.002 -0.001
0.001 0.000 0.000

atensor 11 C
0.207 -0.595 -0.154
-0.595 0.224 0.142
-0.154 0.142 0.408
-0.001 0.002 -0.001
0.004 -0.002 0.001
-0.001 0.000 0.000

atensor 12 C
0.207 0.595 -0.154
0.595 0.224 -0.142
-0.154 -0.142 0.408
-0.001 -0.002 -0.001
-0.004 -0.002 -0.001
-0.001 0.000 0.000

atensor 13 C
1.511 0.799 0.149
0.799 0.400 0.042
0.149 0.042 -0.420
0.003 0.006 0.001
0.005 -0.002 0.000
0.001 -0.002 0.001

atensor 14 C
1.511 -0.799 0.149
-0.799 0.400 -0.042
0.149 -0.042 -0.420
0.003 -0.006 0.001
-0.005 -0.002 0.000
0.001 0.002 0.001

atensor 15 C
1.511 -0.799 -0.149
-0.799 0.400 0.042
-0.149 0.042 -0.420

0.003 -0.006 -0.001
-0.005 -0.002 0.000
-0.001 -0.002 0.001

atensor 16 C
1.511 0.799 -0.149
0.799 0.400 -0.042
-0.149 -0.042 -0.420
0.003 0.006 -0.001
0.005 -0.002 0.000
-0.001 0.002 0.001

atensor 17 C
-0.112 0.242 0.049
0.242 -0.105 0.014
0.049 0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.112 -0.242 0.049
-0.242 -0.105 -0.014
0.049 -0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.112 -0.242 -0.049
-0.242 -0.105 0.014
-0.049 0.014 -0.336
0.001 -0.001 0.000
-0.002 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.112 0.242 -0.049
0.242 -0.105 -0.014
-0.049 -0.014 -0.336
0.001 0.001 0.000
0.002 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.199 -0.132 0.028
-0.132 0.311 -0.017
0.028 -0.017 0.076
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.199 0.132 0.028
0.132 0.311 0.017
0.028 0.017 0.076
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.639 0.086 -0.011
0.086 0.799 0.023
-0.011 0.023 0.831
0.002 -0.001 0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 26 C
1.639 -0.086 -0.011
-0.086 0.799 -0.023
-0.011 -0.023 0.831
0.002 0.001 0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 27 C
1.639 -0.086 0.011
-0.086 0.799 0.023
0.011 0.023 0.831
0.002 0.001 -0.001
0.000 -0.012 0.001
0.000 0.001 -0.001

atensor 28 C
1.639 0.086 0.011
0.086 0.799 -0.023
0.011 -0.023 0.831
0.002 -0.001 -0.001
0.000 -0.012 -0.001
0.000 -0.001 -0.001

atensor 29 C
0.282 0.110 0.044
0.110 0.190 0.053
0.044 0.053 0.095
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.282 -0.110 0.044
-0.110 0.190 -0.053
0.044 -0.053 0.095
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.282 -0.110 -0.044
-0.110 0.190 0.053
-0.044 0.053 0.095
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.282 0.110 -0.044
0.110 0.190 -0.053
-0.044 -0.053 0.095
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.013 0.093 -0.001
0.093 0.041 -0.019
-0.001 -0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.013 -0.093 -0.001

-0.093 0.041 0.019
-0.001 0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.013 -0.093 0.001
-0.093 0.041 -0.019
0.001 -0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.013 0.093 0.001
0.093 0.041 0.019
0.001 0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.033 0.085 0.032
0.085 0.010 0.012
0.032 0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.033 -0.085 0.032
-0.085 0.011 -0.012
0.032 -0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.033 -0.085 -0.032
-0.085 0.011 0.012
-0.032 0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.033 0.085 -0.032
0.085 0.011 -0.012
-0.032 -0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.043 0.045 -0.010
0.045 0.045 0.020
-0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.043 -0.045 -0.010
-0.045 0.045 -0.020
-0.010 -0.020 -0.025
0.000 0.000 0.000

0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.043 -0.045 0.010
-0.045 0.045 0.020
0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.043 0.045 0.010
0.045 0.045 -0.020
0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.176 0.408 0.068
0.408 1.085 0.236
0.068 0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 0.002
0.000 0.000 -0.001

atensor 48 H
-0.176 -0.408 0.068
-0.408 1.085 -0.236
0.068 -0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 49 H
-0.176 -0.408 -0.068
-0.408 1.085 0.236
-0.068 0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 0.002
0.000 0.000 -0.001

atensor 50 H
-0.176 0.408 -0.068
0.408 1.085 -0.236
-0.068 -0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 51 H
-0.112 0.622 -0.191
0.622 0.452 -0.314
-0.191 -0.314 -0.411
-0.001 0.005 -0.001
0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 52 H
-0.112 -0.622 -0.191
-0.622 0.452 0.314
-0.191 0.314 -0.411
-0.001 -0.005 -0.001
-0.005 0.004 0.002
0.000 0.001 -0.001

atensor 53 H
-0.112 -0.622 0.191
-0.622 0.452 -0.314
0.191 -0.314 -0.411
-0.001 -0.005 0.001
-0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 54 H
-0.112 0.622 0.191
0.622 0.452 0.314
0.191 0.314 -0.411
-0.001 0.005 0.001
0.005 0.004 0.002
0.000 0.001 -0.001

atensor 55 H
0.262 0.457 0.389
0.457 -0.111 0.250
0.389 0.250 -0.224
0.002 0.003 0.002
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.262 -0.457 0.389
-0.457 -0.111 -0.250
0.389 -0.250 -0.224
0.002 -0.003 0.002
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.262 -0.457 -0.389
-0.457 -0.111 0.250
-0.389 0.250 -0.224
0.002 -0.003 -0.002
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.262 0.457 -0.389
0.457 -0.111 -0.250
-0.389 -0.250 -0.224
0.002 0.003 -0.002
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.022 0.234 -0.051
0.234 0.160 -0.071
-0.051 -0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.022 -0.234 -0.051
-0.234 0.160 0.071
-0.051 0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.022 -0.234 0.051
-0.234 0.160 -0.071

0.051 -0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.022 0.234 0.051
0.234 0.160 0.071
0.051 0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.282 0.433 0.042
0.433 -0.062 0.017
0.042 0.017 -0.242
0.006 0.002 0.001
0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 64 H
1.282 -0.433 0.042
-0.433 -0.062 -0.017
0.042 -0.017 -0.242
0.006 -0.002 0.001
-0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 65 H
1.282 -0.433 -0.042
-0.433 -0.062 0.017
-0.042 0.017 -0.242
0.006 -0.002 -0.001
-0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 66 H
1.282 0.433 -0.042
0.433 -0.062 -0.017
-0.042 -0.017 -0.242
0.006 0.002 -0.001
0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 67 H
0.124 0.201 0.098
0.201 0.018 0.074
0.098 0.074 -0.100
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.124 -0.201 0.098
-0.201 0.018 -0.074
0.098 -0.074 -0.100
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.124 -0.201 -0.098
-0.201 0.018 0.074
-0.098 0.074 -0.100
0.001 -0.001 -0.001
-0.001 0.000 0.001

0.000 0.000 0.000

atensor 70 H
0.124 0.201 -0.098
0.201 0.018 -0.074
-0.098 -0.074 -0.100
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.039 0.173 0.008
0.173 0.044 0.014
0.008 0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.039 -0.173 0.008
-0.173 0.044 -0.014
0.008 -0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.039 -0.173 -0.008
-0.173 0.044 0.014
-0.008 0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.039 0.173 -0.008
0.173 0.044 -0.014
-0.008 -0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-219.798 -16.527 0.247
-16.527 -304.533 -32.628
0.247 -32.628 -81.387
261.916 -3.867 -0.977
-3.867 258.311 4.277
-0.977 4.277 222.786

orbtensor 2 C
-219.798 16.527 0.247
16.527 -304.533 32.628
0.247 32.628 -81.387
261.916 3.867 -0.977
3.867 258.311 -4.277
-0.977 -4.277 222.786

orbtensor 3 C
-219.798 16.527 -0.247
16.527 -304.533 -32.628
-0.247 -32.628 -81.387
261.916 3.867 0.977
3.867 258.310 4.277
0.977 4.277 222.786

orbtensor 4 C

```
-219.798  -16.527  -0.247
-16.527  -304.533  32.628
-0.247   32.628  -81.387
261.916  -3.867   0.977
-3.867  258.310  -4.277
0.977   -4.277  222.786
```

```
orbtensor 5 C
-277.637  -8.681   1.112
-8.681  -296.230  -21.902
1.112  -21.902  -106.798
270.796   2.396  -0.261
2.396  265.805   3.262
-0.261   3.262  228.473
```

```
orbtensor 6 C
-277.637   8.681   1.112
8.681  -296.230   21.902
1.112   21.902  -106.798
270.796  -2.396  -0.261
-2.396  265.805  -3.262
-0.261  -3.262  228.473
```

```
orbtensor 7 C
-277.637   8.681  -1.112
8.681  -296.230  -21.902
-1.112  -21.902  -106.798
270.796  -2.396   0.261
-2.396  265.805   3.262
0.261   3.262  228.473
```

```
orbtensor 8 C
-277.637  -8.681  -1.112
-8.681  -296.230   21.902
-1.112   21.902  -106.798
270.795   2.396   0.261
2.396  265.805  -3.262
0.261  -3.262  228.472
```

```
orbtensor 9 C
-249.491  -12.396   9.928
-12.396  -252.178  -11.080
9.928  -11.080  -66.308
262.720   0.698  -0.426
0.698  262.961   0.841
-0.426   0.841  217.221
```

```
orbtensor 10 C
-249.491   12.396   9.928
12.396  -252.178   11.080
9.928   11.080  -66.308
262.720  -0.698  -0.426
-0.698  262.961  -0.841
-0.426  -0.841  217.221
```

```
orbtensor 11 C
-249.491   12.396  -9.928
12.396  -252.177  -11.080
-9.928  -11.080  -66.308
262.720  -0.698   0.426
-0.698  262.961   0.841
0.426   0.841  217.221
```

```
orbtensor 12 C
-249.491  -12.396  -9.928
-12.396  -252.178   11.080
-9.928   11.080  -66.309
```

262.720 0.698 0.426
0.698 262.961 -0.841
0.426 -0.841 217.221

orbtensor 13 C
-287.722 -4.323 23.246
-4.323 -284.314 -1.604
23.246 -1.604 -96.264
266.346 2.106 -1.575
2.106 270.495 0.787
-1.575 0.787 228.491

orbtensor 14 C
-287.722 4.323 23.246
4.323 -284.314 1.604
23.246 1.604 -96.264
266.346 -2.106 -1.575
-2.106 270.495 -0.787
-1.575 -0.787 228.490

orbtensor 15 C
-287.722 4.323 -23.246
4.323 -284.314 -1.604
-23.246 -1.604 -96.264
266.346 -2.106 1.575
-2.106 270.495 0.787
1.575 0.787 228.491

orbtensor 16 C
-287.722 -4.323 -23.246
-4.323 -284.314 1.604
-23.246 1.604 -96.264
266.346 2.106 1.575
2.106 270.495 -0.787
1.575 -0.787 228.490

orbtensor 17 C
-220.425 -107.042 -56.328
-107.042 -218.711 58.919
-56.328 58.919 -212.040
253.905 14.332 9.928
14.332 253.937 -9.939
9.928 -9.939 249.814

orbtensor 18 C
-220.425 107.042 -56.328
107.042 -218.711 -58.919
-56.328 -58.919 -212.039
253.905 -14.332 9.928
-14.332 253.937 9.939
9.928 9.939 249.814

orbtensor 19 C
-220.425 107.042 56.328
107.042 -218.711 58.919
56.328 58.919 -212.039
253.905 -14.332 -9.928
-14.332 253.937 -9.939
-9.928 -9.939 249.814

orbtensor 20 C
-220.425 -107.042 56.328
-107.042 -218.711 -58.919
56.328 -58.919 -212.039
253.905 14.332 -9.928
14.332 253.937 9.939
-9.928 9.939 249.814

orbtensor 23 C
-199.906 69.053 90.890
69.053 -165.240 49.179
90.890 49.179 -256.951
246.835 -14.813 -6.186
-14.813 250.029 -13.239
-6.186 -13.239 249.087

orbtensor 24 C
-199.906 -69.053 90.890
-69.053 -165.240 -49.179
90.890 -49.179 -256.951
246.835 14.813 -6.186
14.813 250.029 13.239
-6.186 13.239 249.087

orbtensor 25 C
-298.442 -13.808 34.429
-13.808 -218.228 5.976
34.429 5.976 -82.159
259.034 -4.004 -3.491
-4.004 261.073 1.044
-3.491 1.044 222.064

orbtensor 26 C
-298.442 13.808 34.428
13.808 -218.228 -5.976
34.428 -5.976 -82.159
259.034 4.004 -3.491
4.004 261.073 -1.044
-3.491 -1.044 222.063

orbtensor 27 C
-298.442 13.808 -34.428
13.808 -218.228 5.976
-34.428 5.976 -82.159
259.034 4.004 3.491
4.004 261.073 1.044
3.491 1.044 222.064

orbtensor 28 C
-298.442 -13.808 -34.429
-13.808 -218.228 -5.976
-34.429 -5.976 -82.159
259.034 -4.004 3.491
-4.004 261.073 -1.044
3.491 -1.044 222.063

orbtensor 29 C
-164.718 -67.087 -50.667
-67.087 -194.781 89.679
-50.667 89.679 -257.645
249.703 14.878 13.275
14.878 246.374 -6.421
13.275 -6.421 248.699

orbtensor 30 C
-164.718 67.087 -50.667
67.087 -194.781 -89.679
-50.667 -89.679 -257.645
249.703 -14.878 13.275
-14.878 246.374 6.421
13.275 6.421 248.699

orbtensor 31 C
-164.718 67.087 50.667

67.087 -194.781 89.679
50.667 89.679 -257.645
249.703 -14.878 -13.275
-14.878 246.374 -6.421
-13.275 -6.421 248.699

orbtensor 32 C
-164.718 -67.087 50.667
-67.087 -194.781 -89.679
50.667 -89.679 -257.645
249.703 14.878 -13.275
14.878 246.374 6.421
-13.275 6.421 248.699

orbtensor 33 C
-153.672 -69.730 -47.690
-69.730 -193.105 99.196
-47.690 99.196 -227.627
246.002 15.537 10.651
15.537 243.801 -9.560
10.651 -9.560 245.187

orbtensor 34 C
-153.671 69.730 -47.690
69.730 -193.105 -99.195
-47.690 -99.195 -227.627
246.002 -15.537 10.651
-15.537 243.801 9.560
10.651 9.560 245.187

orbtensor 35 C
-153.672 69.730 47.690
69.730 -193.105 99.196
47.690 99.196 -227.627
246.002 -15.537 -10.651
-15.537 243.801 -9.560
-10.651 -9.560 245.187

orbtensor 36 C
-153.672 -69.730 47.690
-69.730 -193.105 -99.195
47.690 -99.195 -227.627
246.002 15.537 -10.651
15.537 243.801 9.560
-10.651 9.560 245.187

orbtensor 37 C
-196.533 -72.009 -98.674
-72.009 -153.027 45.511
-98.674 45.511 -225.023
244.261 15.417 9.376
15.417 246.022 -10.752
9.376 -10.752 245.480

orbtensor 38 C
-196.532 72.009 -98.674
72.009 -153.027 -45.511
-98.674 -45.511 -225.023
244.261 -15.417 9.376
-15.417 246.022 10.752
9.376 10.752 245.480

orbtensor 39 C
-196.533 72.009 98.674
72.009 -153.027 45.511
98.674 45.511 -225.023
244.261 -15.417 -9.376

-15.417 246.022 -10.752
-9.376 -10.752 245.480

orbtensor 40 C
-196.532 -72.009 98.674
-72.009 -153.027 -45.511
98.674 -45.511 -225.023
244.261 15.417 -9.376
15.417 246.022 10.752
-9.376 10.752 245.480

orbtensor 41 C
-204.564 -113.874 -52.184
-113.874 -205.269 55.381
-52.184 55.381 -176.283
245.765 12.118 10.812
12.118 245.491 -10.918
10.812 -10.918 249.845

orbtensor 42 C
-204.564 113.874 -52.184
113.874 -205.269 -55.381
-52.184 -55.381 -176.283
245.765 -12.118 10.812
-12.118 245.491 10.918
10.812 10.918 249.845

orbtensor 43 C
-204.564 113.874 52.184
113.874 -205.269 55.381
52.184 55.381 -176.283
245.765 -12.118 -10.812
-12.118 245.491 -10.918
-10.812 -10.918 249.845

orbtensor 44 C
-204.564 -113.874 52.184
-113.874 -205.269 -55.381
52.184 -55.381 -176.283
245.765 12.118 -10.812
12.118 245.491 10.918
-10.812 10.918 249.845

orbtensor 47 H
-3.904 -8.144 -1.426
-8.144 -14.349 -1.398
-1.426 -1.398 -6.636
35.327 4.785 -0.718
4.785 35.620 2.424
-0.718 2.424 18.611

orbtensor 48 H
-3.904 8.144 -1.426
8.144 -14.349 1.398
-1.426 1.398 -6.636
35.327 -4.785 -0.718
-4.785 35.620 -2.424
-0.718 -2.424 18.611

orbtensor 49 H
-3.904 8.144 1.426
8.144 -14.349 -1.398
1.426 -1.398 -6.636
35.327 -4.785 0.718
-4.785 35.620 2.424
0.718 2.424 18.611

orbtensor 50 H
-3.904 -8.144 1.426
-8.144 -14.349 1.398
1.426 1.398 -6.636
35.327 4.785 0.718
4.785 35.620 -2.424
0.718 -2.424 18.610

orbtensor 51 H
-8.946 -1.757 -10.027
-1.757 -2.727 -2.562
-10.027 -2.562 -14.002
32.448 4.565 5.548
4.565 27.218 -3.800
5.548 -3.800 33.438

orbtensor 52 H
-8.946 1.757 -10.027
1.757 -2.727 2.562
-10.027 2.562 -14.002
32.448 -4.565 5.548
-4.565 27.218 3.800
5.548 3.800 33.438

orbtensor 53 H
-8.946 1.757 10.027
1.757 -2.727 -2.562
10.027 -2.562 -14.002
32.448 -4.565 -5.548
-4.565 27.218 -3.800
-5.548 -3.800 33.438

orbtensor 54 H
-8.946 -1.757 10.027
-1.757 -2.727 2.562
10.027 2.562 -14.002
32.448 4.565 -5.548
4.565 27.218 3.800
-5.548 3.800 33.438

orbtensor 55 H
-2.506 -1.223 2.043
-1.223 -8.569 9.911
2.043 9.911 -14.864
27.164 4.054 4.168
4.054 32.304 -5.470
4.168 -5.470 34.066

orbtensor 56 H
-2.506 1.223 2.043
1.223 -8.569 -9.911
2.043 -9.911 -14.864
27.164 -4.054 4.168
-4.054 32.304 5.470
4.168 5.470 34.066

orbtensor 57 H
-2.506 1.223 -2.043
1.223 -8.569 9.911
-2.043 9.911 -14.864
27.164 -4.054 -4.168
-4.054 32.304 -5.470
-4.168 -5.470 34.066

orbtensor 58 H
-2.506 -1.223 -2.043
-1.223 -8.569 -9.911

-2.043	-9.911	-14.864
27.164	4.054	-4.168
4.054	32.304	5.470
-4.168	5.470	34.065

orbtensor 59 H

-1.987	-1.121	0.424
-1.121	-9.304	7.715
0.424	7.715	-12.819
27.008	3.716	0.808
3.716	32.777	-9.059
0.808	-9.059	33.948

orbtensor 60 H

-1.987	1.121	0.424
1.121	-9.304	-7.715
0.424	-7.715	-12.819
27.008	-3.716	0.808
-3.716	32.777	9.059
0.808	9.059	33.948

orbtensor 61 H

-1.987	1.121	-0.424
1.121	-9.304	7.715
-0.424	7.715	-12.819
27.008	-3.716	-0.808
-3.716	32.777	-9.059
-0.808	-9.059	33.948

orbtensor 62 H

-1.987	-1.121	-0.424
-1.121	-9.304	-7.715
-0.424	-7.715	-12.819
27.008	3.716	-0.808
3.716	32.777	9.059
-0.808	9.059	33.948

orbtensor 63 H

-14.105	-7.983	1.406
-7.983	-3.770	1.604
1.406	1.604	-6.565
36.312	4.833	-1.935
4.833	35.277	0.704
-1.935	0.704	18.411

orbtensor 64 H

-14.105	7.983	1.406
7.983	-3.770	-1.604
1.406	-1.604	-6.565
36.312	-4.833	-1.935
-4.833	35.277	-0.704
-1.935	-0.704	18.410

orbtensor 65 H

-14.105	7.983	-1.406
7.983	-3.770	1.604
-1.406	1.604	-6.565
36.312	-4.833	1.935
-4.833	35.277	0.704
1.935	0.704	18.411

orbtensor 66 H

-14.105	-7.983	-1.406
-7.983	-3.770	-1.604
-1.406	-1.604	-6.565
36.312	4.833	1.935
4.833	35.277	-0.704

1.935 -0.704 18.410

orbtensor 67 H

-9.687 -1.440 -7.764
-1.440 -2.083 -0.777
-7.764 -0.777 -12.439
33.174 3.940 9.038
3.940 27.077 -0.565
9.038 -0.565 33.619

orbtensor 68 H

-9.687 1.440 -7.764
1.440 -2.083 0.777
-7.764 0.777 -12.439
33.174 -3.940 9.038
-3.940 27.077 0.565
9.038 0.565 33.619

orbtensor 69 H

-9.687 1.440 7.764
1.440 -2.083 -0.777
7.764 -0.777 -12.438
33.174 -3.940 -9.038
-3.940 27.077 -0.565
-9.038 -0.565 33.619

orbtensor 70 H

-9.687 -1.440 7.764
-1.440 -2.083 0.777
7.764 0.777 -12.439
33.174 3.940 -9.038
3.940 27.077 0.565
-9.038 0.565 33.619

orbtensor 71 H

-10.488 -8.892 0.319
-8.892 -10.747 0.152
0.319 0.152 -3.201
33.752 9.672 1.584
9.672 33.908 -2.015
1.584 -2.015 26.546

orbtensor 72 H

-10.488 8.892 0.319
8.892 -10.747 -0.152
0.319 -0.152 -3.201
33.752 -9.672 1.584
-9.672 33.908 2.015
1.584 2.015 26.546

orbtensor 73 H

-10.488 8.892 -0.319
8.892 -10.747 0.152
-0.319 0.152 -3.201
33.752 -9.672 -1.584
-9.672 33.908 -2.015
-1.584 -2.015 26.546

orbtensor 74 H

-10.488 -8.892 -0.319
-8.892 -10.747 -0.152
-0.319 -0.152 -3.201
33.752 9.672 -1.584
9.672 33.908 2.015
-1.584 2.015 26.546

gtensor (ppt)

```

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9737	45.76500	-1177.19575	0.00000	-1177.19575	-1131.43075
2	C	0.9737	45.76500	-1177.19575	0.00000	-1177.19575	-1131.43075
3	C	0.9737	45.76467	-1177.19575	0.00000	-1177.19575	-1131.43108
4	C	0.9737	45.76467	-1177.19575	0.00000	-1177.19575	-1131.43108
5	C	0.9183	28.13633	-1110.29589	-0.00000	-1110.29589	-1082.15956
6	C	0.9183	28.13633	-1110.29589	-0.00000	-1110.29589	-1082.15956
7	C	0.9183	28.13633	-1110.29589	-0.00000	-1110.29589	-1082.15956
8	C	0.9183	28.13567	-1110.29589	-0.00000	-1110.29589	-1082.16022
9	C	0.2787	58.30833	-336.91737	0.00000	-336.91737	-278.60904
10	C	0.2787	58.30833	-336.91737	0.00000	-336.91737	-278.60904
11	C	0.2787	58.30867	-336.91737	0.00000	-336.91737	-278.60871
12	C	0.2787	58.30800	-336.91737	0.00000	-336.91737	-278.60937
13	C	0.4977	32.34400	-601.69574	0.00000	-601.69574	-569.35174
14	C	0.4977	32.34367	-601.69574	0.00000	-601.69574	-569.35207
15	C	0.4977	32.34400	-601.69574	0.00000	-601.69574	-569.35174
16	C	0.4977	32.34367	-601.69574	0.00000	-601.69574	-569.35207
17	C	-0.1840	35.49333	222.46219	-0.00000	222.46219	257.95552
18	C	-0.1840	35.49367	222.46219	-0.00000	222.46219	257.95586
19	C	-0.1840	35.49367	222.46219	-0.00000	222.46219	257.95586
20	C	-0.1840	35.49367	222.46219	-0.00000	222.46219	257.95586
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1957	41.28467	-236.56758	-0.00000	-236.56758	-195.28291
24	C	0.1957	41.28467	-236.56758	-0.00000	-236.56758	-195.28291
25	C	1.0860	47.78067	-1313.01053	0.00000	-1313.01053	-1265.22986
26	C	1.0860	47.78033	-1313.01053	0.00000	-1313.01053	-1265.23020
27	C	1.0860	47.78067	-1313.01053	0.00000	-1313.01053	-1265.22986
28	C	1.0860	47.78033	-1313.01053	0.00000	-1313.01053	-1265.23020
29	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
30	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
31	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
32	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
33	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
34	C	0.0003	53.52900	-0.40301	-0.00000	-0.40301	53.12599
35	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
36	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
A Average		0.7080	30.24000	-855.99581	-0.00000	-855.99581	-825.75581
B Average		1.0298	46.77267	-1245.10314	0.00000	-1245.10314	-1198.33047
M Average		0.2787	58.30833	-336.91737	0.00000	-336.91737	-278.60904

=====
FeL5-saddled-HS-STO-PBE0-No-PSOSO

Temperature: 303

Spin: 2.5

atensor 1 C

0.687 0.061 0.014

0.061 1.476 0.115

0.014 0.115 0.766

0.000 0.000 0.000

0.000 0.000 0.000
0.000 0.000 0.000

atensor 2 C
0.687 -0.061 0.014
-0.061 1.476 -0.115
0.014 -0.115 0.766
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
0.687 -0.061 -0.014
-0.061 1.476 0.115
-0.014 0.115 0.766
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 C
0.687 0.061 -0.014
0.061 1.476 -0.115
-0.014 -0.115 0.766
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.790 0.802 0.105
0.802 1.951 0.315
0.105 0.315 0.010
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 C
0.790 -0.802 0.105
-0.802 1.951 -0.315
0.105 -0.315 0.010
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
0.790 -0.802 -0.105
-0.802 1.951 0.315
-0.105 0.315 0.010
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 C
0.790 0.802 -0.105
0.802 1.951 -0.315
-0.105 -0.315 0.010
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.207 0.595 0.154
0.595 0.224 0.142
0.154 0.142 0.408
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 C
0.207 -0.595 0.154
-0.595 0.224 -0.142
0.154 -0.142 0.408
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.207 -0.595 -0.154
-0.595 0.224 0.142
-0.154 0.142 0.408
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 C
0.207 0.595 -0.154
0.595 0.224 -0.142
-0.154 -0.142 0.408
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
1.511 0.799 0.149
0.799 0.400 0.042
0.149 0.042 -0.420
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 C
1.511 -0.799 0.149
-0.799 0.400 -0.042
0.149 -0.042 -0.420
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
1.511 -0.799 -0.149
-0.799 0.400 0.042
-0.149 0.042 -0.420
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 C
1.511 0.799 -0.149
0.799 0.400 -0.042
-0.149 -0.042 -0.420
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
-0.112 0.242 0.049
0.242 -0.105 0.014
0.049 0.014 -0.336
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.112 -0.242 0.049
-0.242 -0.105 -0.014

0.049 -0.014 -0.336
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.112 -0.242 -0.049
-0.242 -0.105 0.014
-0.049 0.014 -0.336
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.112 0.242 -0.049
0.242 -0.105 -0.014
-0.049 -0.014 -0.336
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.199 -0.132 0.028
-0.132 0.311 -0.017
0.028 -0.017 0.076
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 C
0.199 0.132 0.028
0.132 0.311 0.017
0.028 0.017 0.076
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 C
1.639 0.086 -0.011
0.086 0.799 0.023
-0.011 0.023 0.831
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 C
1.639 -0.086 -0.011
-0.086 0.799 -0.023
-0.011 -0.023 0.831
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 C
1.639 -0.086 0.011
-0.086 0.799 0.023
0.011 0.023 0.831
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 C
1.639 0.086 0.011
0.086 0.799 -0.023
0.011 -0.023 0.831
0.000 0.000 0.000
0.000 0.000 0.000

0.000 0.000 0.000

atensor 29 C
0.282 0.110 0.044
0.110 0.190 0.053
0.044 0.053 0.095
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.282 -0.110 0.044
-0.110 0.190 -0.053
0.044 -0.053 0.095
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.282 -0.110 -0.044
-0.110 0.190 0.053
-0.044 0.053 0.095
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.282 0.110 -0.044
0.110 0.190 -0.053
-0.044 -0.053 0.095
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.013 0.093 -0.001
0.093 0.041 -0.019
-0.001 -0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.013 -0.093 -0.001
-0.093 0.041 0.019
-0.001 0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.013 -0.093 0.001
-0.093 0.041 -0.019
0.001 -0.019 -0.053
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.013 0.093 0.001
0.093 0.041 0.019
0.001 0.019 -0.053
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C

0.033 0.085 0.032
0.085 0.010 0.012
0.032 0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.033 -0.085 0.032
-0.085 0.011 -0.012
0.032 -0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.033 -0.085 -0.032
-0.085 0.011 0.012
-0.032 0.012 -0.045
0.000 0.000 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.033 0.085 -0.032
0.085 0.011 -0.012
-0.032 -0.012 -0.045
0.000 0.000 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.043 0.045 -0.010
0.045 0.045 0.020
-0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.043 -0.045 -0.010
-0.045 0.045 -0.020
-0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.043 -0.045 0.010
-0.045 0.045 0.020
0.010 0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.043 0.045 0.010
0.045 0.045 -0.020
0.010 -0.020 -0.025
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.176 0.408 0.068
0.408 1.085 0.236
0.068 0.236 -0.317

-0.004 0.001 0.000
0.002 0.006 0.002
0.000 0.000 -0.001

atensor 48 H
-0.176 -0.408 0.068
-0.408 1.085 -0.236
0.068 -0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 49 H
-0.176 -0.408 -0.068
-0.408 1.085 0.236
-0.068 0.236 -0.317
-0.004 -0.001 0.000
-0.002 0.006 0.002
0.000 0.000 -0.001

atensor 50 H
-0.176 0.408 -0.068
0.408 1.085 -0.236
-0.068 -0.236 -0.317
-0.004 0.001 0.000
0.002 0.006 -0.002
0.000 0.000 -0.001

atensor 51 H
-0.112 0.622 -0.191
0.622 0.452 -0.314
-0.191 -0.314 -0.411
-0.001 0.005 -0.001
0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 52 H
-0.112 -0.622 -0.191
-0.622 0.452 0.314
-0.191 0.314 -0.411
-0.001 -0.005 -0.001
-0.005 0.004 0.002
0.000 0.001 -0.001

atensor 53 H
-0.112 -0.622 0.191
-0.622 0.452 -0.314
0.191 -0.314 -0.411
-0.001 -0.005 0.001
-0.005 0.004 -0.002
0.000 -0.001 -0.001

atensor 54 H
-0.112 0.622 0.191
0.622 0.452 0.314
0.191 0.314 -0.411
-0.001 0.005 0.001
0.005 0.004 0.002
0.000 0.001 -0.001

atensor 55 H
0.262 0.457 0.389
0.457 -0.111 0.250
0.389 0.250 -0.224
0.002 0.003 0.002
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.262 -0.457 0.389
-0.457 -0.111 -0.250
0.389 -0.250 -0.224
0.002 -0.003 0.002
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.262 -0.457 -0.389
-0.457 -0.111 0.250
-0.389 0.250 -0.224
0.002 -0.003 -0.002
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.262 0.457 -0.389
0.457 -0.111 -0.250
-0.389 -0.250 -0.224
0.002 0.003 -0.002
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.022 0.234 -0.051
0.234 0.160 -0.071
-0.051 -0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.022 -0.234 -0.051
-0.234 0.160 0.071
-0.051 0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.022 -0.234 0.051
-0.234 0.160 -0.071
0.051 -0.071 -0.134
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.022 0.234 0.051
0.234 0.160 0.071
0.051 0.071 -0.134
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.282 0.433 0.042
0.433 -0.062 0.017
0.042 0.017 -0.242
0.006 0.002 0.001
0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 64 H
1.282 -0.433 0.042

-0.433 -0.062 -0.017
0.042 -0.017 -0.242
0.006 -0.002 0.001
-0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 65 H
1.282 -0.433 -0.042
-0.433 -0.062 0.017
-0.042 0.017 -0.242
0.006 -0.002 -0.001
-0.002 -0.005 0.001
0.000 0.000 -0.001

atensor 66 H
1.282 0.433 -0.042
0.433 -0.062 -0.017
-0.042 -0.017 -0.242
0.006 0.002 -0.001
0.002 -0.005 -0.001
0.000 0.000 -0.001

atensor 67 H
0.124 0.201 0.098
0.201 0.018 0.074
0.098 0.074 -0.100
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.124 -0.201 0.098
-0.201 0.018 -0.074
0.098 -0.074 -0.100
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.124 -0.201 -0.098
-0.201 0.018 0.074
-0.098 0.074 -0.100
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.124 0.201 -0.098
0.201 0.018 -0.074
-0.098 -0.074 -0.100
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.039 0.173 0.008
0.173 0.044 0.014
0.008 0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.039 -0.173 0.008
-0.173 0.044 -0.014
0.008 -0.014 -0.137
0.000 -0.001 0.000

-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.039 -0.173 -0.008
-0.173 0.044 0.014
-0.008 0.014 -0.137
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.039 0.173 -0.008
0.173 0.044 -0.014
-0.008 -0.014 -0.137
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-219.798 -16.527 0.247
-16.527 -304.533 -32.628
0.247 -32.628 -81.387
261.916 -3.867 -0.977
-3.867 258.311 4.277
-0.977 4.277 222.786

orbtensor 2 C
-219.798 16.527 0.247
16.527 -304.533 32.628
0.247 32.628 -81.387
261.916 3.867 -0.977
3.867 258.311 -4.277
-0.977 -4.277 222.786

orbtensor 3 C
-219.798 16.527 -0.247
16.527 -304.533 -32.628
-0.247 -32.628 -81.387
261.916 3.867 0.977
3.867 258.310 4.277
0.977 4.277 222.786

orbtensor 4 C
-219.798 -16.527 -0.247
-16.527 -304.533 32.628
-0.247 32.628 -81.387
261.916 -3.867 0.977
-3.867 258.310 -4.277
0.977 -4.277 222.786

orbtensor 5 C
-277.637 -8.681 1.112
-8.681 -296.230 -21.902
1.112 -21.902 -106.798
270.796 2.396 -0.261
2.396 265.805 3.262
-0.261 3.262 228.473

orbtensor 6 C
-277.637 8.681 1.112
8.681 -296.230 21.902
1.112 21.902 -106.798
270.796 -2.396 -0.261
-2.396 265.805 -3.262
-0.261 -3.262 228.473

orbtensor 7 C
-277.637 8.681 -1.112
8.681 -296.230 -21.902
-1.112 -21.902 -106.798
270.796 -2.396 0.261
-2.396 265.805 3.262
0.261 3.262 228.473

orbtensor 8 C
-277.637 -8.681 -1.112
-8.681 -296.230 21.902
-1.112 21.902 -106.798
270.795 2.396 0.261
2.396 265.805 -3.262
0.261 -3.262 228.472

orbtensor 9 C
-249.491 -12.396 9.928
-12.396 -252.178 -11.080
9.928 -11.080 -66.308
262.720 0.698 -0.426
0.698 262.961 0.841
-0.426 0.841 217.221

orbtensor 10 C
-249.491 12.396 9.928
12.396 -252.178 11.080
9.928 11.080 -66.308
262.720 -0.698 -0.426
-0.698 262.961 -0.841
-0.426 -0.841 217.221

orbtensor 11 C
-249.491 12.396 -9.928
12.396 -252.177 -11.080
-9.928 -11.080 -66.308
262.720 -0.698 0.426
-0.698 262.961 0.841
0.426 0.841 217.221

orbtensor 12 C
-249.491 -12.396 -9.928
-12.396 -252.178 11.080
-9.928 11.080 -66.309
262.720 0.698 0.426
0.698 262.961 -0.841
0.426 -0.841 217.221

orbtensor 13 C
-287.722 -4.323 23.246
-4.323 -284.314 -1.604
23.246 -1.604 -96.264
266.346 2.106 -1.575
2.106 270.495 0.787
-1.575 0.787 228.491

orbtensor 14 C
-287.722 4.323 23.246
4.323 -284.314 1.604
23.246 1.604 -96.264
266.346 -2.106 -1.575
-2.106 270.495 -0.787
-1.575 -0.787 228.490

orbtensor 15 C
-287.722 4.323 -23.246
4.323 -284.314 -1.604

-23.246 -1.604 -96.264
266.346 -2.106 1.575
-2.106 270.495 0.787
1.575 0.787 228.491

orbtensor 16 C
-287.722 -4.323 -23.246
-4.323 -284.314 1.604
-23.246 1.604 -96.264
266.346 2.106 1.575
2.106 270.495 -0.787
1.575 -0.787 228.490

orbtensor 17 C
-220.425 -107.042 -56.328
-107.042 -218.711 58.919
-56.328 58.919 -212.040
253.905 14.332 9.928
14.332 253.937 -9.939
9.928 -9.939 249.814

orbtensor 18 C
-220.425 107.042 -56.328
107.042 -218.711 -58.919
-56.328 -58.919 -212.039
253.905 -14.332 9.928
-14.332 253.937 9.939
9.928 9.939 249.814

orbtensor 19 C
-220.425 107.042 56.328
107.042 -218.711 58.919
56.328 58.919 -212.039
253.905 -14.332 -9.928
-14.332 253.937 -9.939
-9.928 -9.939 249.814

orbtensor 20 C
-220.425 -107.042 56.328
-107.042 -218.711 -58.919
56.328 -58.919 -212.039
253.905 14.332 -9.928
14.332 253.937 9.939
-9.928 9.939 249.814

orbtensor 23 C
-199.906 69.053 90.890
69.053 -165.240 49.179
90.890 49.179 -256.951
246.835 -14.813 -6.186
-14.813 250.029 -13.239
-6.186 -13.239 249.087

orbtensor 24 C
-199.906 -69.053 90.890
-69.053 -165.240 -49.179
90.890 -49.179 -256.951
246.835 14.813 -6.186
14.813 250.029 13.239
-6.186 13.239 249.087

orbtensor 25 C
-298.442 -13.808 34.429
-13.808 -218.228 5.976
34.429 5.976 -82.159
259.034 -4.004 -3.491
-4.004 261.073 1.044

```

-3.491    1.044    222.064

orbtensor 26 C
-298.442    13.808    34.428
13.808   -218.228    -5.976
34.428    -5.976   -82.159
259.034     4.004    -3.491
4.004   261.073    -1.044
-3.491    -1.044    222.063

orbtensor 27 C
-298.442    13.808   -34.428
13.808   -218.228     5.976
-34.428     5.976   -82.159
259.034     4.004     3.491
4.004   261.073     1.044
3.491     1.044    222.064

orbtensor 28 C
-298.442   -13.808   -34.429
-13.808   -218.228    -5.976
-34.429    -5.976   -82.159
259.034    -4.004     3.491
-4.004   261.073    -1.044
3.491    -1.044    222.063

orbtensor 29 C
-164.718   -67.087   -50.667
-67.087  -194.781    89.679
-50.667    89.679  -257.645
249.703    14.878    13.275
14.878   246.374   -6.421
13.275   -6.421   248.699

orbtensor 30 C
-164.718     67.087   -50.667
67.087  -194.781   -89.679
-50.667   -89.679  -257.645
249.703   -14.878    13.275
-14.878   246.374     6.421
13.275     6.421   248.699

orbtensor 31 C
-164.718     67.087    50.667
67.087  -194.781    89.679
50.667    89.679  -257.645
249.703   -14.878   -13.275
-14.878   246.374   -6.421
-13.275   -6.421   248.699

orbtensor 32 C
-164.718   -67.087    50.667
-67.087  -194.781   -89.679
50.667   -89.679  -257.645
249.703    14.878   -13.275
14.878   246.374     6.421
-13.275     6.421   248.699

orbtensor 33 C
-153.672   -69.730   -47.690
-69.730  -193.105    99.196
-47.690    99.196  -227.627
246.002    15.537    10.651
15.537   243.801   -9.560
10.651   -9.560   245.187

orbtensor 34 C

```

-153.671 69.730 -47.690
69.730 -193.105 -99.195
-47.690 -99.195 -227.627
246.002 -15.537 10.651
-15.537 243.801 9.560
10.651 9.560 245.187

orbtensor 35 C
-153.672 69.730 47.690
69.730 -193.105 99.196
47.690 99.196 -227.627
246.002 -15.537 -10.651
-15.537 243.801 -9.560
-10.651 -9.560 245.187

orbtensor 36 C
-153.672 -69.730 47.690
-69.730 -193.105 -99.195
47.690 -99.195 -227.627
246.002 15.537 -10.651
15.537 243.801 9.560
-10.651 9.560 245.187

orbtensor 37 C
-196.533 -72.009 -98.674
-72.009 -153.027 45.511
-98.674 45.511 -225.023
244.261 15.417 9.376
15.417 246.022 -10.752
9.376 -10.752 245.480

orbtensor 38 C
-196.532 72.009 -98.674
72.009 -153.027 -45.511
-98.674 -45.511 -225.023
244.261 -15.417 9.376
-15.417 246.022 10.752
9.376 10.752 245.480

orbtensor 39 C
-196.533 72.009 98.674
72.009 -153.027 45.511
98.674 45.511 -225.023
244.261 -15.417 -9.376
-15.417 246.022 -10.752
-9.376 -10.752 245.480

orbtensor 40 C
-196.532 -72.009 98.674
-72.009 -153.027 -45.511
98.674 -45.511 -225.023
244.261 15.417 -9.376
15.417 246.022 10.752
-9.376 10.752 245.480

orbtensor 41 C
-204.564 -113.874 -52.184
-113.874 -205.269 55.381
-52.184 55.381 -176.283
245.765 12.118 10.812
12.118 245.491 -10.918
10.812 -10.918 249.845

orbtensor 42 C
-204.564 113.874 -52.184
113.874 -205.269 -55.381
-52.184 -55.381 -176.283

245.765	-12.118	10.812
-12.118	245.491	10.918
10.812	10.918	249.845

orbtensor 43 C

-204.564	113.874	52.184
113.874	-205.269	55.381
52.184	55.381	-176.283
245.765	-12.118	-10.812
-12.118	245.491	-10.918
-10.812	-10.918	249.845

orbtensor 44 C

-204.564	-113.874	52.184
-113.874	-205.269	-55.381
52.184	-55.381	-176.283
245.765	12.118	-10.812
12.118	245.491	10.918
-10.812	10.918	249.845

orbtensor 47 H

-3.904	-8.144	-1.426
-8.144	-14.349	-1.398
-1.426	-1.398	-6.636
35.327	4.785	-0.718
4.785	35.620	2.424
-0.718	2.424	18.611

orbtensor 48 H

-3.904	8.144	-1.426
8.144	-14.349	1.398
-1.426	1.398	-6.636
35.327	-4.785	-0.718
-4.785	35.620	-2.424
-0.718	-2.424	18.611

orbtensor 49 H

-3.904	8.144	1.426
8.144	-14.349	-1.398
1.426	-1.398	-6.636
35.327	-4.785	0.718
-4.785	35.620	2.424
0.718	2.424	18.611

orbtensor 50 H

-3.904	-8.144	1.426
-8.144	-14.349	1.398
1.426	1.398	-6.636
35.327	4.785	0.718
4.785	35.620	-2.424
0.718	-2.424	18.610

orbtensor 51 H

-8.946	-1.757	-10.027
-1.757	-2.727	-2.562
-10.027	-2.562	-14.002
32.448	4.565	5.548
4.565	27.218	-3.800
5.548	-3.800	33.438

orbtensor 52 H

-8.946	1.757	-10.027
1.757	-2.727	2.562
-10.027	2.562	-14.002
32.448	-4.565	5.548
-4.565	27.218	3.800
5.548	3.800	33.438

orbtensor 53 H
-8.946 1.757 10.027
1.757 -2.727 -2.562
10.027 -2.562 -14.002
32.448 -4.565 -5.548
-4.565 27.218 -3.800
-5.548 -3.800 33.438

orbtensor 54 H
-8.946 -1.757 10.027
-1.757 -2.727 2.562
10.027 2.562 -14.002
32.448 4.565 -5.548
4.565 27.218 3.800
-5.548 3.800 33.438

orbtensor 55 H
-2.506 -1.223 2.043
-1.223 -8.569 9.911
2.043 9.911 -14.864
27.164 4.054 4.168
4.054 32.304 -5.470
4.168 -5.470 34.066

orbtensor 56 H
-2.506 1.223 2.043
1.223 -8.569 -9.911
2.043 -9.911 -14.864
27.164 -4.054 4.168
-4.054 32.304 5.470
4.168 5.470 34.066

orbtensor 57 H
-2.506 1.223 -2.043
1.223 -8.569 9.911
-2.043 9.911 -14.864
27.164 -4.054 -4.168
-4.054 32.304 -5.470
-4.168 -5.470 34.066

orbtensor 58 H
-2.506 -1.223 -2.043
-1.223 -8.569 -9.911
-2.043 -9.911 -14.864
27.164 4.054 -4.168
4.054 32.304 5.470
-4.168 5.470 34.065

orbtensor 59 H
-1.987 -1.121 0.424
-1.121 -9.304 7.715
0.424 7.715 -12.819
27.008 3.716 0.808
3.716 32.777 -9.059
0.808 -9.059 33.948

orbtensor 60 H
-1.987 1.121 0.424
1.121 -9.304 -7.715
0.424 -7.715 -12.819
27.008 -3.716 0.808
-3.716 32.777 9.059
0.808 9.059 33.948

orbtensor 61 H
-1.987 1.121 -0.424

1.121	-9.304	7.715
-0.424	7.715	-12.819
27.008	-3.716	-0.808
-3.716	32.777	-9.059
-0.808	-9.059	33.948

orbtensor 62 H

-1.987	-1.121	-0.424
-1.121	-9.304	-7.715
-0.424	-7.715	-12.819
27.008	3.716	-0.808
3.716	32.777	9.059
-0.808	9.059	33.948

orbtensor 63 H

-14.105	-7.983	1.406
-7.983	-3.770	1.604
1.406	1.604	-6.565
36.312	4.833	-1.935
4.833	35.277	0.704
-1.935	0.704	18.411

orbtensor 64 H

-14.105	7.983	1.406
7.983	-3.770	-1.604
1.406	-1.604	-6.565
36.312	-4.833	-1.935
-4.833	35.277	-0.704
-1.935	-0.704	18.410

orbtensor 65 H

-14.105	7.983	-1.406
7.983	-3.770	1.604
-1.406	1.604	-6.565
36.312	-4.833	1.935
-4.833	35.277	0.704
1.935	0.704	18.411

orbtensor 66 H

-14.105	-7.983	-1.406
-7.983	-3.770	-1.604
-1.406	-1.604	-6.565
36.312	4.833	1.935
4.833	35.277	-0.704
1.935	-0.704	18.410

orbtensor 67 H

-9.687	-1.440	-7.764
-1.440	-2.083	-0.777
-7.764	-0.777	-12.439
33.174	3.940	9.038
3.940	27.077	-0.565
9.038	-0.565	33.619

orbtensor 68 H

-9.687	1.440	-7.764
1.440	-2.083	0.777
-7.764	0.777	-12.439
33.174	-3.940	9.038
-3.940	27.077	0.565
9.038	0.565	33.619

orbtensor 69 H

-9.687	1.440	7.764
1.440	-2.083	-0.777
7.764	-0.777	-12.438
33.174	-3.940	-9.038

-3.940 27.077 -0.565
 -9.038 -0.565 33.619

orbtensor 70 H
 -9.687 -1.440 7.764
 -1.440 -2.083 0.777
 7.764 0.777 -12.439
 33.174 3.940 -9.038
 3.940 27.077 0.565
 -9.038 0.565 33.619

orbtensor 71 H
 -10.488 -8.892 0.319
 -8.892 -10.747 0.152
 0.319 0.152 -3.201
 33.752 9.672 1.584
 9.672 33.908 -2.015
 1.584 -2.015 26.546

orbtensor 72 H
 -10.488 8.892 0.319
 8.892 -10.747 -0.152
 0.319 -0.152 -3.201
 33.752 -9.672 1.584
 -9.672 33.908 2.015
 1.584 2.015 26.546

orbtensor 73 H
 -10.488 8.892 -0.319
 8.892 -10.747 0.152
 -0.319 0.152 -3.201
 33.752 -9.672 -1.584
 -9.672 33.908 -2.015
 -1.584 -2.015 26.546

orbtensor 74 H
 -10.488 -8.892 -0.319
 -8.892 -10.747 -0.152
 -0.319 -0.152 -3.201
 33.752 9.672 -1.584
 9.672 33.908 2.015
 -1.584 2.015 26.546

gtensor (ppt)
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

averaging
 A Average:5,6,7,8,13,14,15,16
 B Average:1,2,3,4,25,26,27,28
 M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9763	45.76500	-1180.41984	0.00000	-1180.41984	-1134.65484
2	C	0.9763	45.76500	-1180.41984	0.00000	-1180.41984	-1134.65484
3	C	0.9763	45.76467	-1180.41984	0.00000	-1180.41984	-1134.65517
4	C	0.9763	45.76467	-1180.41984	0.00000	-1180.41984	-1134.65517
5	C	0.9170	28.13633	-1108.68384	-0.00000	-1108.68384	-1080.54751
6	C	0.9170	28.13633	-1108.68384	-0.00000	-1108.68384	-1080.54751
7	C	0.9170	28.13633	-1108.68384	-0.00000	-1108.68384	-1080.54751

8	C	0.9170	28.13567	-1108.68384	-0.00000	-1108.68384	-1080.54818
9	C	0.2797	58.30833	-338.12641	0.00000	-338.12641	-279.81807
10	C	0.2797	58.30833	-338.12641	0.00000	-338.12641	-279.81807
11	C	0.2797	58.30867	-338.12641	0.00000	-338.12641	-279.81774
12	C	0.2797	58.30800	-338.12641	0.00000	-338.12641	-279.81841
13	C	0.4970	32.34400	-600.88972	0.00000	-600.88972	-568.54572
14	C	0.4970	32.34367	-600.88972	0.00000	-600.88972	-568.54605
15	C	0.4970	32.34400	-600.88972	0.00000	-600.88972	-568.54572
16	C	0.4970	32.34367	-600.88972	0.00000	-600.88972	-568.54605
17	C	-0.1843	35.49333	222.86520	-0.00000	222.86520	258.35853
18	C	-0.1843	35.49367	222.86520	-0.00000	222.86520	258.35887
19	C	-0.1843	35.49367	222.86520	-0.00000	222.86520	258.35887
20	C	-0.1843	35.49367	222.86520	-0.00000	222.86520	258.35887
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1953	41.28467	-236.16457	-0.00000	-236.16457	-194.87990
24	C	0.1953	41.28467	-236.16457	-0.00000	-236.16457	-194.87990
25	C	1.0897	47.78067	-1317.44365	0.00000	-1317.44365	-1269.66299
26	C	1.0897	47.78033	-1317.44365	0.00000	-1317.44365	-1269.66332
27	C	1.0897	47.78067	-1317.44365	0.00000	-1317.44365	-1269.66299
28	C	1.0897	47.78033	-1317.44365	0.00000	-1317.44365	-1269.66332
29	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
30	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
31	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
32	C	0.1890	42.54400	-228.50736	-0.00000	-228.50736	-185.96336
33	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
34	C	0.0003	53.52900	-0.40301	-0.00000	-0.40301	53.12599
35	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
36	C	0.0003	53.52867	-0.40301	-0.00000	-0.40301	53.12566
A Average		0.7070	30.24000	-854.78678	-0.00000	-854.78678	-824.54678
B Average		1.0330	46.77267	-1248.93175	0.00000	-1248.93175	-1202.15908
M Average		0.2797	58.30833	-338.12641	0.00000	-338.12641	-279.81807

=====
FeL5-saddled-HS-STO-PBE0-No-ZORA
Temperature: 303
Spin: 2.5

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	0.9843	45.89533	-1190.09211	0.00000	-1190.09211	-1144.19678
2	C	0.9843	45.89500	-1190.09211	0.00000	-1190.09211	-1144.19711
3	C	0.9843	45.89500	-1190.09211	0.00000	-1190.09211	-1144.19711
4	C	0.9843	45.89500	-1190.09211	0.00000	-1190.09211	-1144.19711
5	C	0.8783	28.22900	-1061.93454	-0.00000	-1061.93454	-1033.70554
6	C	0.8783	28.22900	-1061.93454	-0.00000	-1061.93454	-1033.70554
7	C	0.8783	28.22900	-1061.93454	-0.00000	-1061.93454	-1033.70554
8	C	0.8783	28.22900	-1061.93454	-0.00000	-1061.93454	-1033.70554
9	C	0.3083	58.33500	-372.78537	0.00000	-372.78537	-314.45037
10	C	0.3083	58.33500	-372.78537	0.00000	-372.78537	-314.45037
11	C	0.3083	58.33467	-372.78537	0.00000	-372.78537	-314.45070
12	C	0.3083	58.33467	-372.78537	0.00000	-372.78537	-314.45070
13	C	0.4610	32.48433	-557.36451	-0.00000	-557.36451	-524.88017
14	C	0.4610	32.48400	-557.36451	-0.00000	-557.36451	-524.88051
15	C	0.4610	32.48400	-557.36451	-0.00000	-557.36451	-524.88051
16	C	0.4610	32.48400	-557.36451	-0.00000	-557.36451	-524.88051
17	C	-0.1970	35.66067	238.17963	-0.00000	238.17963	273.84029
18	C	-0.1970	35.66100	238.17963	-0.00000	238.17963	273.84063
19	C	-0.1970	35.66067	238.17963	-0.00000	238.17963	273.84029
20	C	-0.1970	35.66067	238.17963	-0.00000	238.17963	273.84029
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2077	41.47033	-251.07599	0.00000	-251.07599	-209.60565

24	C	0.2077	41.47033	-251.07599	0.00000	-251.07599	-209.60565
25	C	1.0980	47.99367	-1327.51893	-0.00000	-1327.51893	-1279.52527
26	C	1.0980	47.99367	-1327.51893	-0.00000	-1327.51893	-1279.52527
27	C	1.0980	47.99367	-1327.51893	-0.00000	-1327.51893	-1279.52527
28	C	1.0980	47.99367	-1327.51893	-0.00000	-1327.51893	-1279.52527
29	C	0.2013	42.72933	-243.41877	0.00000	-243.41877	-200.68944
30	C	0.2013	42.72933	-243.41877	0.00000	-243.41877	-200.68944
31	C	0.2013	42.72933	-243.41877	0.00000	-243.41877	-200.68944
32	C	0.2013	42.72900	-243.41877	0.00000	-243.41877	-200.68977
33	C	0.0000	53.69367	0.00000	-0.00000	-0.00000	53.69367
34	C	0.0000	53.69367	0.00000	-0.00000	-0.00000	53.69367
35	C	0.0000	53.69367	0.00000	-0.00000	-0.00000	53.69367
36	C	0.0000	53.69367	0.00000	-0.00000	-0.00000	53.69367
A Average		0.6697	30.35654	-809.64953	-0.00000	-809.64953	-779.29298
B Average		1.0412	46.94438	-1258.80552	-0.00000	-1258.80552	-1211.86115
M Average		0.3083	58.33483	-372.78537	0.00000	-372.78537	-314.45054

=====
 FeL5-planar-LS-STO-PBE0-Full-Finite
 Temperature: 303
 Spin: 1.5

atensor 1 C
 -0.611 0.169 -0.023
 0.169 -0.279 0.292
 -0.023 0.292 -0.308
 -0.031 -0.003 -0.001
 0.007 0.010 0.002
 -0.002 0.001 -0.001

atensor 2 C
 -0.614 -0.170 -0.021
 -0.170 -0.282 -0.292
 -0.021 -0.292 -0.311
 -0.031 0.003 -0.001
 -0.007 0.010 -0.002
 -0.002 -0.001 -0.001

atensor 3 C
 -0.614 -0.170 0.021
 -0.170 -0.282 0.292
 0.021 0.292 -0.311
 -0.031 0.003 0.001
 -0.007 0.010 0.002
 0.002 0.001 -0.001

atensor 4 C
 -0.611 0.169 0.023
 0.169 -0.279 -0.292
 0.023 -0.292 -0.308
 -0.031 -0.003 0.001
 0.007 0.010 -0.002
 0.002 -0.001 -0.001

atensor 5 C
 -1.430 0.447 0.228
 0.447 -0.451 0.534
 0.228 0.534 -1.407
 -0.013 0.014 0.007
 0.034 0.000 0.006
 0.005 0.000 0.000

atensor 6 C
 -1.425 -0.450 0.229
 -0.450 -0.446 -0.533
 0.229 -0.533 -1.406

-0.013 -0.014 0.007
-0.034 0.000 -0.006
0.005 0.000 0.000

atensor 7 C
-1.425 -0.450 -0.229
-0.450 -0.446 0.533
-0.229 0.533 -1.406
-0.013 -0.014 -0.007
-0.034 0.000 0.006
-0.005 0.000 0.000

atensor 8 C
-1.430 0.447 -0.228
0.447 -0.451 -0.534
-0.228 -0.534 -1.407
-0.013 0.014 -0.007
0.034 0.000 -0.006
-0.005 0.000 0.000

atensor 9 C
0.429 0.641 0.348
0.641 0.448 -0.002
0.348 -0.002 0.422
0.004 0.008 0.002
0.002 0.002 0.002
0.004 0.001 -0.002

atensor 10 C
0.430 -0.643 0.348
-0.643 0.447 0.003
0.348 0.003 0.419
0.004 -0.008 0.002
-0.002 0.002 -0.002
0.004 -0.002 -0.003

atensor 11 C
0.430 -0.643 -0.348
-0.643 0.447 -0.003
-0.348 -0.003 0.420
0.004 -0.008 -0.002
-0.002 0.002 0.002
-0.004 0.002 -0.003

atensor 12 C
0.429 0.641 -0.348
0.641 0.448 0.002
-0.348 0.002 0.422
0.004 0.008 -0.002
0.002 0.002 -0.002
-0.004 -0.001 -0.002

atensor 13 C
-0.188 0.489 0.459
0.489 -1.320 0.161
0.459 0.161 -1.324
0.006 0.029 0.008
0.011 -0.007 0.004
0.001 -0.001 -0.001

atensor 14 C
-0.184 -0.490 0.457
-0.490 -1.320 -0.161
0.457 -0.161 -1.324
0.006 -0.029 0.008
-0.011 -0.007 -0.004
0.001 0.001 -0.001

atensor 15 C
-0.184 -0.490 -0.458
-0.490 -1.320 0.161
-0.458 0.161 -1.324
0.006 -0.029 -0.008
-0.011 -0.007 0.004
-0.001 -0.001 -0.001

atensor 16 C
-0.188 0.489 -0.459
0.489 -1.320 -0.161
-0.459 -0.161 -1.324
0.006 0.029 -0.008
0.011 -0.007 -0.004
-0.001 0.000 -0.001

atensor 17 C
-0.032 0.233 0.063
0.233 -0.028 0.037
0.063 0.037 -0.238
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.001

atensor 18 C
-0.031 -0.233 0.061
-0.233 -0.028 -0.036
0.062 -0.036 -0.238
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.001

atensor 19 C
-0.031 -0.233 -0.062
-0.233 -0.028 0.036
-0.062 0.036 -0.238
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 20 C
-0.032 0.233 -0.063
0.233 -0.028 -0.037
-0.063 -0.037 -0.238
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 23 C
0.170 -0.137 0.013
-0.137 0.256 -0.002
0.013 -0.002 0.049
0.000 -0.003 0.000
-0.003 0.002 0.000
0.000 0.000 -0.001

atensor 24 C
0.170 0.136 0.012
0.136 0.256 0.001
0.012 0.001 0.049
0.000 0.003 0.000
0.003 0.002 0.000
0.000 0.000 -0.001

atensor 25 C
-0.046 0.157 0.290

0.157 -0.545 -0.031
0.290 -0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 0.001
0.002 0.002 -0.001

atensor 26 C
-0.043 -0.158 0.290
-0.158 -0.544 0.031
0.290 0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 -0.001
0.002 -0.002 -0.001

atensor 27 C
-0.042 -0.158 -0.290
-0.158 -0.544 -0.031
-0.290 -0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 0.001
-0.002 0.002 -0.001

atensor 28 C
-0.046 0.157 -0.290
0.157 -0.545 0.031
-0.290 0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 -0.001
-0.002 -0.002 -0.001

atensor 29 C
0.216 0.108 0.057
0.108 0.139 0.057
0.057 0.057 0.066
0.001 0.002 0.001
0.002 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.216 -0.108 0.057
-0.108 0.140 -0.056
0.057 -0.056 0.065
0.001 -0.002 0.001
-0.002 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.216 -0.108 -0.057
-0.108 0.139 0.056
-0.057 0.056 0.065
0.001 -0.002 -0.001
-0.002 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.216 0.108 -0.057
0.108 0.139 -0.057
-0.057 -0.057 0.066
0.001 0.002 -0.001
0.002 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.012 0.089 0.005
0.089 0.037 -0.008
0.005 -0.008 -0.053
0.000 0.002 0.000

0.002 0.001 0.000
0.000 0.000 0.000

atensor 34 C
0.012 -0.089 0.004
-0.089 0.037 0.008
0.004 0.008 -0.052
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 35 C
0.012 -0.089 -0.004
-0.089 0.037 -0.008
-0.004 -0.008 -0.053
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 36 C
0.012 0.089 -0.005
0.089 0.037 0.008
-0.005 0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

orbtensor 1 C
-222.362 -17.574 -3.419
-17.574 -303.468 -44.049
-3.419 -44.049 -89.081
261.494 -4.060 -0.927
-4.060 258.056 5.856
-0.927 5.856 222.641

orbtensor 2 C
-219.822 18.349 -4.355
18.349 -305.492 43.384
-4.355 43.384 -94.639
261.477 4.036 -1.132
4.036 258.063 -5.866
-1.132 -5.866 222.651

orbtensor 3 C
-225.433 15.568 1.835
15.568 -302.935 -43.705
1.835 -43.705 -89.026
261.477 4.037 1.130
4.037 258.062 5.867
1.130 5.867 222.651

orbtensor 4 C
-221.119 -17.507 4.230
-17.507 -302.720 45.591
4.230 45.591 -88.361
261.495 -4.060 0.924
-4.060 258.056 -5.854
0.924 -5.854 222.641

orbtensor 5 C
-279.271 -8.927 1.192
-8.927 -296.354 -34.255
1.192 -34.255 -98.567
270.944 2.019 0.384
2.019 266.007 4.911
0.384 4.911 229.406

orbtensor 6 C
-281.853 9.014 1.600
9.014 -296.140 38.319
1.600 38.319 -100.112
270.956 -2.042 0.214
-2.042 266.021 -4.864
0.214 -4.864 229.412

orbtensor 7 C
-281.804 10.260 2.305
10.260 -296.000 -36.410
2.305 -36.410 -99.234
270.953 -2.041 -0.216
-2.041 266.019 4.867
-0.216 4.867 229.411

orbtensor 8 C
-282.637 -9.705 -1.646
-9.705 -295.389 36.978
-1.646 36.978 -98.897
270.944 2.019 -0.386
2.019 266.007 -4.910
-0.386 -4.910 229.405

orbtensor 9 C
-260.028 -16.678 3.762
-16.678 -257.763 -19.947
3.762 -19.947 -74.490
262.817 0.533 0.714
0.533 262.805 2.897
0.714 2.897 217.367

orbtensor 10 C
-258.075 16.776 2.631
16.776 -256.206 18.355
2.631 18.355 -74.760
262.813 -0.548 0.564
-0.548 262.836 -2.743
0.564 -2.743 217.353

orbtensor 11 C
-259.053 16.505 -2.329
16.505 -255.102 -18.427
-2.329 -18.427 -72.893
262.814 -0.548 -0.565
-0.548 262.834 2.745
-0.565 2.745 217.353

orbtensor 12 C
-259.644 -17.318 -2.280
-17.318 -256.759 21.007
-2.280 21.007 -72.020
262.815 0.535 -0.716
0.535 262.805 -2.893
-0.716 -2.893 217.365

orbtensor 13 C
-300.220 -10.661 19.115
-10.661 -283.140 -20.629
19.115 -20.629 -95.205
266.508 1.899 -0.234
1.899 271.118 1.929
-0.234 1.929 229.103

orbtensor 14 C
-299.361 9.261 21.554
9.261 -283.447 19.255

21.554	19.255	-96.204
266.514	-1.897	-0.276
-1.897	271.134	-1.751
-0.276	-1.751	229.095

orbtensor 15 C

-299.760	8.706	-19.523
8.706	-283.319	-18.030
-19.523	-18.030	-92.955
266.515	-1.898	0.276
-1.898	271.134	1.754
0.276	1.754	229.097

orbtensor 16 C

-298.786	-9.278	-19.658
-9.278	-284.538	21.670
-19.658	21.670	-91.661
266.508	1.899	0.234
1.899	271.117	-1.927
0.234	-1.927	229.102

orbtensor 17 C

-218.501	-108.469	-55.365
-108.469	-227.945	45.796
-55.365	45.796	-222.958
252.344	14.870	10.140
14.870	254.107	-8.811
10.140	-8.811	250.685

orbtensor 18 C

-218.900	107.498	-56.534
107.498	-227.150	-48.087
-56.534	-48.087	-221.677
252.384	-14.898	10.055
-14.898	254.036	8.849
10.055	8.849	250.744

orbtensor 19 C

-218.219	106.533	56.357
106.533	-228.161	46.389
56.357	46.389	-222.751
252.389	-14.894	-10.058
-14.894	254.040	-8.853
-10.058	-8.853	250.737

orbtensor 20 C

-218.946	-108.296	56.214
-108.296	-227.903	-47.905
56.214	-47.905	-224.610
252.347	14.866	-10.142
14.866	254.113	8.812
-10.142	8.812	250.685

orbtensor 23 C

-193.282	69.991	87.172
69.991	-174.808	46.914
87.172	46.914	-267.542
245.744	-15.658	-6.098
-15.658	250.614	-12.114
-6.098	-12.114	249.517

orbtensor 24 C

-193.222	-69.996	86.837
-69.996	-172.025	-47.389
86.837	-47.389	-271.332
245.733	15.657	-6.175
15.657	250.707	12.079

```

-6.175    12.079    249.419

orbtensor 25 C
-312.221  -16.100    23.996
-16.100  -225.653    13.001
23.996    13.001   -81.517
258.847   -4.032   -2.131
-4.032    261.430    1.193
-2.131     1.193    221.940

orbtensor 26 C
-308.989   15.571    25.399
15.571  -226.116   -12.374
25.399  -12.374   -80.989
258.850    4.042   -2.118
4.042    261.444   -0.981
-2.118   -0.981    221.933

orbtensor 27 C
-313.381   15.811   -26.469
15.811  -220.610    13.579
-26.469   13.579   -81.968
258.850    4.041    2.119
4.041    261.444    0.984
2.119     0.984    221.933

orbtensor 28 C
-308.357  -15.213   -25.179
-15.213  -225.153   -14.558
-25.179  -14.558   -81.711
258.848   -4.031    2.131
-4.031    261.430   -1.191
2.131    -1.191    221.940

orbtensor 29 C
-160.338  -73.027   -45.228
-73.027  -206.610    86.383
-45.228   86.383  -262.083
247.892   14.962   13.429
14.962   246.764   -5.422
13.429   -5.422   250.413

orbtensor 30 C
-165.514   73.669   -43.051
73.669  -205.408   -87.458
-43.051  -87.458  -265.541
247.934  -15.018   13.369
-15.018   246.724    5.428
13.369    5.428   250.400

orbtensor 31 C
-167.692   72.526   43.555
72.526  -206.088   85.026
43.555   85.026  -266.954
247.944  -15.014  -13.372
-15.014   246.724   -5.433
-13.372   -5.433   250.394

orbtensor 32 C
-164.600  -73.589   47.121
-73.589  -204.736   -87.419
47.121  -87.419  -264.097
247.893   14.959  -13.432
14.959   246.767    5.424
-13.432    5.424   250.410

orbtensor 33 C

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-149.589  -78.558  -42.356
-78.558  -202.581  95.781
-42.356   95.781  -230.527
244.309   15.917   10.859
15.917   244.341  -8.472
10.859   -8.472   246.523

```

```

orbtensor 34 C
-149.043   78.293  -46.608
78.293  -204.735  -96.494
-46.608  -96.494  -229.922
244.325  -15.956   10.786
-15.956  244.272   8.486
10.786   8.486   246.559

```

```

orbtensor 35 C
-148.248   78.835   44.117
78.835  -199.365   96.060
44.117   96.060  -229.443
244.333  -15.953  -10.789
-15.953  244.271  -8.492
-10.789  -8.492   246.549

```

```

orbtensor 36 C
-150.734  -76.802   43.924
-76.802  -200.921  -94.823
43.924  -94.823  -230.340
244.310   15.915  -10.862
15.915  244.344   8.473
-10.862   8.473   246.519

```

```

gtensor (ppt)
-0.151   0.000   0.000
0.000  -0.156   0.000
0.000   0.000  -0.239
38.654  -1.060  -1.414
-1.060  40.681  -2.586
-1.414  -2.586  17.581

```

```

zfstensor (cm-1)
2.389903  -0.007870   0.003689
-0.007870   1.548798  -0.005294
0.003689  -0.005294  125.987003

```

```

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4067	42.42667	205.69997	9.91391	215.61387	258.04054
2	C	-0.4097	40.74600	207.21743	9.62661	216.84404	257.59004
3	C	-0.4097	41.59867	207.21743	9.85778	217.07520	258.67387
4	C	-0.4067	43.33067	205.69997	9.70322	215.40319	258.73386
5	C	-1.1003	30.72167	556.57016	-31.54519	525.02497	555.74663
6	C	-1.0967	29.42800	554.71548	-32.40445	522.31103	551.73903
7	C	-1.0967	29.78167	554.71548	-32.10230	522.61318	552.39485
8	C	-1.1003	29.81100	556.57016	-32.05078	524.51938	554.33038
9	C	0.4343	50.23600	-219.69431	-1.27348	-220.96778	-170.73178
10	C	0.4330	51.32033	-219.01988	-1.79468	-220.81457	-169.49423
11	C	0.4333	51.98433	-219.18849	-1.87934	-221.06783	-169.08349
12	C	0.4343	51.52067	-219.69431	-1.42500	-221.11931	-169.59864
13	C	-0.9447	29.38800	477.83091	-37.97796	439.85294	469.24094
14	C	-0.9433	29.24367	477.15648	-38.43164	438.72484	467.96851
15	C	-0.9433	30.23733	477.15648	-38.50909	438.64739	468.88472

16	C	-0.9447	30.58067	477.83091	-38.30029	439.53062	470.11129
17	C	-0.0983	29.24400	49.73893	-14.30462	35.43431	64.67831
18	C	-0.0980	29.81233	49.57032	-14.45769	35.11263	64.92496
19	C	-0.0980	29.34500	49.57032	-14.45771	35.11261	64.45761
20	C	-0.0983	28.56200	49.73893	-14.36023	35.37869	63.94069
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1587	36.74767	-80.25671	-11.38373	-91.64044	-54.89277
24	C	0.1587	36.42667	-80.25671	-11.32882	-91.58553	-55.15886
25	C	-0.3323	40.94200	168.10071	-5.10427	162.99644	203.93844
26	C	-0.3307	42.04433	167.25768	-5.21090	162.04678	204.09111
27	C	-0.3303	42.08933	167.08907	-5.39261	161.69646	203.78579
28	C	-0.3323	42.33233	168.10071	-5.20820	162.89251	205.22484
29	C	0.1403	38.67933	-70.98335	-7.60024	-78.58358	-39.90425
30	C	0.1403	36.19833	-70.98335	-7.78895	-78.77230	-42.57397
31	C	0.1400	34.77600	-70.81474	-7.73642	-78.55116	-43.77516
32	C	0.1403	37.21233	-70.98335	-7.66910	-78.65245	-41.44012
33	C	-0.0010	50.82533	0.50582	-5.31307	-4.80725	46.01809
34	C	-0.0007	50.48533	0.33721	-5.27433	-4.93712	45.54821
35	C	-0.0010	52.69900	0.50582	-5.35023	-4.84441	47.85459
36	C	-0.0010	51.05933	0.50582	-5.30919	-4.80337	46.25596
A Average		-1.0212	29.89900	516.56826	-35.16521	481.40304	511.30204
B Average		-0.3698	41.93875	187.04787	2.27319	189.32106	231.25981
M Average		0.4337	51.26533	-219.39925	-1.59312	-220.99237	-169.72704

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FeL5-planar-LS-STO-PBE0-Full-ORCA

Temperature: 303

Spin: 1.5

atensor 1 C

-0.611 0.169 -0.023
0.169 -0.279 0.292
-0.023 0.292 -0.308
-0.031 -0.003 -0.001
0.007 0.010 0.002
-0.002 0.001 -0.001

atensor 2 C

-0.614 -0.170 -0.021
-0.170 -0.282 -0.292
-0.021 -0.292 -0.311
-0.031 0.003 -0.001
-0.007 0.010 -0.002
-0.002 -0.001 -0.001

atensor 3 C

-0.614 -0.170 0.021
-0.170 -0.282 0.292
0.021 0.292 -0.311
-0.031 0.003 0.001
-0.007 0.010 0.002
0.002 0.001 -0.001

atensor 4 C

-0.611 0.169 0.023
0.169 -0.279 -0.292
0.023 -0.292 -0.308
-0.031 -0.003 0.001
0.007 0.010 -0.002
0.002 -0.001 -0.001

atensor 5 C

-1.430 0.447 0.228
0.447 -0.451 0.534
0.228 0.534 -1.407

-0.013 0.014 0.007
0.034 0.000 0.006
0.005 0.000 0.000

atensor 6 C
-1.425 -0.450 0.229
-0.450 -0.446 -0.533
0.229 -0.533 -1.406
-0.013 -0.014 0.007
-0.034 0.000 -0.006
0.005 0.000 0.000

atensor 7 C
-1.425 -0.450 -0.229
-0.450 -0.446 0.533
-0.229 0.533 -1.406
-0.013 -0.014 -0.007
-0.034 0.000 0.006
-0.005 0.000 0.000

atensor 8 C
-1.430 0.447 -0.228
0.447 -0.451 -0.534
-0.228 -0.534 -1.407
-0.013 0.014 -0.007
0.034 0.000 -0.006
-0.005 0.000 0.000

atensor 9 C
0.429 0.641 0.348
0.641 0.449 -0.002
0.348 -0.002 0.422
0.004 0.008 0.002
0.002 0.002 0.002
0.004 0.001 -0.002

atensor 10 C
0.431 -0.643 0.348
-0.643 0.447 0.003
0.348 0.003 0.419
0.004 -0.008 0.002
-0.002 0.002 -0.002
0.004 -0.002 -0.003

atensor 11 C
0.431 -0.643 -0.348
-0.643 0.447 -0.003
-0.348 -0.003 0.420
0.004 -0.008 -0.002
-0.002 0.002 0.002
-0.004 0.002 -0.003

atensor 12 C
0.429 0.641 -0.348
0.641 0.449 0.002
-0.348 0.002 0.422
0.004 0.008 -0.002
0.002 0.002 -0.002
-0.004 -0.001 -0.002

atensor 13 C
-0.188 0.489 0.459
0.489 -1.320 0.161
0.459 0.161 -1.324
0.006 0.029 0.008
0.011 -0.007 0.004
0.001 -0.001 -0.001

atensor 14 C
-0.184 -0.490 0.457
-0.490 -1.320 -0.161
0.457 -0.161 -1.324
0.006 -0.029 0.008
-0.011 -0.007 -0.004
0.001 0.001 -0.001

atensor 15 C
-0.184 -0.490 -0.458
-0.490 -1.320 0.161
-0.458 0.161 -1.324
0.006 -0.029 -0.008
-0.011 -0.007 0.004
-0.001 -0.001 -0.001

atensor 16 C
-0.188 0.489 -0.459
0.489 -1.320 -0.161
-0.459 -0.161 -1.324
0.006 0.029 -0.008
0.011 -0.007 -0.004
-0.001 0.000 -0.001

atensor 17 C
-0.032 0.233 0.063
0.233 -0.028 0.037
0.063 0.037 -0.238
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.001

atensor 18 C
-0.031 -0.233 0.061
-0.233 -0.028 -0.036
0.062 -0.036 -0.238
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.001

atensor 19 C
-0.031 -0.233 -0.062
-0.233 -0.028 0.036
-0.062 0.036 -0.238
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 20 C
-0.032 0.233 -0.063
0.233 -0.028 -0.037
-0.063 -0.037 -0.238
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 23 C
0.170 -0.137 0.013
-0.137 0.256 -0.002
0.013 -0.002 0.049
0.000 -0.003 0.000
-0.003 0.002 0.000
0.000 0.000 -0.001

atensor 24 C
0.170 0.136 0.012

0.136 0.256 0.001
0.012 0.001 0.049
0.000 0.003 0.000
0.003 0.002 0.000
0.000 0.000 -0.001

atensor 25 C
-0.046 0.157 0.290
0.157 -0.545 -0.031
0.290 -0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 0.001
0.002 0.002 -0.001

atensor 26 C
-0.043 -0.158 0.290
-0.158 -0.544 0.031
0.290 0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 -0.001
0.002 -0.002 -0.001

atensor 27 C
-0.042 -0.158 -0.290
-0.158 -0.544 -0.031
-0.290 -0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 0.001
-0.002 0.002 -0.001

atensor 28 C
-0.046 0.157 -0.290
0.157 -0.545 0.031
-0.290 0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 -0.001
-0.002 -0.002 -0.001

atensor 29 C
0.216 0.108 0.057
0.108 0.139 0.057
0.057 0.057 0.066
0.001 0.002 0.001
0.002 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.216 -0.108 0.057
-0.108 0.140 -0.056
0.057 -0.056 0.065
0.001 -0.002 0.001
-0.002 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.216 -0.108 -0.057
-0.108 0.140 0.056
-0.057 0.056 0.065
0.001 -0.002 -0.001
-0.002 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.216 0.108 -0.057
0.108 0.139 -0.057
-0.057 -0.057 0.066
0.001 0.002 -0.001

0.002 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.012 0.089 0.005
0.089 0.037 -0.008
0.005 -0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 34 C
0.012 -0.089 0.004
-0.089 0.037 0.008
0.004 0.008 -0.052
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 35 C
0.012 -0.089 -0.004
-0.089 0.037 -0.008
-0.004 -0.008 -0.053
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 36 C
0.012 0.089 -0.005
0.089 0.037 0.008
-0.005 0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 37 C
0.025 0.078 0.036
0.078 0.009 0.020
0.036 0.020 -0.039
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.025 -0.078 0.036
-0.078 0.009 -0.020
0.036 -0.020 -0.039
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.025 -0.078 -0.036
-0.078 0.009 0.020
-0.036 0.020 -0.039
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.025 0.078 -0.036
0.078 0.009 -0.020
-0.036 -0.020 -0.039
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.039 0.045 -0.001
0.045 0.037 0.022
-0.001 0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.039 -0.046 -0.002
-0.046 0.037 -0.021
-0.002 -0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.039 -0.046 0.002
-0.046 0.037 0.021
0.002 0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.039 0.045 0.001
0.045 0.037 -0.022
0.001 -0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.608 0.359 0.031
0.359 0.644 0.299
0.031 0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 0.006
0.000 0.002 -0.004

atensor 48 H
-0.608 -0.360 0.031
-0.360 0.645 -0.297
0.031 -0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 -0.005
0.000 -0.002 -0.004

atensor 49 H
-0.607 -0.360 -0.031
-0.360 0.645 0.297
-0.031 0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 0.005
0.000 0.002 -0.004

atensor 50 H
-0.608 0.359 -0.031
0.359 0.644 -0.299
-0.031 -0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 -0.006
0.000 -0.002 -0.004

atensor 51 H
-0.065 0.641 -0.138
0.641 0.451 -0.222

-0.138 -0.222 -0.426
-0.001 0.012 -0.003
0.012 0.009 -0.004
-0.001 -0.002 -0.004

atensor 52 H
-0.065 -0.643 -0.142
-0.643 0.451 0.227
-0.142 0.227 -0.426
-0.001 -0.012 -0.003
-0.012 0.009 0.004
-0.002 0.002 -0.004

atensor 53 H
-0.065 -0.643 0.141
-0.643 0.451 -0.227
0.141 -0.227 -0.426
-0.001 -0.012 0.003
-0.012 0.009 -0.004
0.002 -0.002 -0.004

atensor 54 H
-0.065 0.641 0.138
0.641 0.451 0.222
0.138 0.222 -0.426
-0.001 0.012 0.003
0.012 0.009 0.004
0.001 0.002 -0.004

atensor 55 H
0.237 0.433 0.408
0.433 -0.123 0.260
0.408 0.260 -0.155
0.005 0.009 0.008
0.009 -0.002 0.005
0.004 0.002 -0.001

atensor 56 H
0.238 -0.434 0.405
-0.434 -0.121 -0.259
0.405 -0.259 -0.158
0.005 -0.009 0.008
-0.009 -0.002 -0.005
0.004 -0.002 -0.001

atensor 57 H
0.238 -0.434 -0.405
-0.434 -0.121 0.259
-0.405 0.259 -0.158
0.005 -0.009 -0.008
-0.009 -0.002 0.005
-0.004 0.002 -0.001

atensor 58 H
0.237 0.433 -0.408
0.433 -0.123 -0.260
-0.408 -0.260 -0.155
0.005 0.009 -0.008
0.009 -0.002 -0.005
-0.004 -0.002 -0.001

atensor 59 H
0.026 0.235 -0.031
0.235 0.151 -0.042
-0.031 -0.042 -0.143
0.000 0.004 -0.001
0.004 0.003 -0.001

0.000 0.000 -0.001

atensor 60 H
0.026 -0.235 -0.032
-0.235 0.151 0.044
-0.032 0.044 -0.143
0.000 -0.004 -0.001
-0.004 0.003 0.001
0.000 0.000 -0.001

atensor 61 H
0.026 -0.235 0.032
-0.235 0.151 -0.044
0.032 -0.044 -0.143
0.000 -0.004 0.001
-0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 62 H
0.026 0.235 0.031
0.235 0.151 0.042
0.031 0.042 -0.143
0.000 0.004 0.001
0.004 0.003 0.001
0.000 0.000 -0.001

atensor 63 H
0.730 0.370 0.145
0.370 -0.621 -0.001
0.145 -0.001 -0.623
0.018 0.008 0.002
0.003 -0.013 0.001
0.001 0.001 -0.005

atensor 64 H
0.733 -0.370 0.143
-0.370 -0.620 0.002
0.143 0.002 -0.622
0.018 -0.008 0.002
-0.003 -0.013 -0.001
0.001 -0.001 -0.005

atensor 65 H
0.733 -0.370 -0.143
-0.370 -0.620 -0.002
-0.143 -0.002 -0.622
0.018 -0.008 -0.002
-0.003 -0.013 0.001
-0.001 0.001 -0.005

atensor 66 H
0.730 0.370 -0.145
0.370 -0.621 0.001
-0.145 0.001 -0.623
0.018 0.008 -0.002
0.003 -0.013 -0.001
-0.001 -0.001 -0.005

atensor 67 H
0.106 0.189 0.114
0.189 0.007 0.087
0.114 0.087 -0.083
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H

0.106 -0.190 0.113
-0.190 0.008 -0.086
0.113 -0.086 -0.084
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.106 -0.190 -0.113
-0.190 0.008 0.086
-0.113 0.086 -0.084
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.106 0.189 -0.114
0.189 0.007 -0.087
-0.114 -0.087 -0.083
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.040 0.166 0.026
0.166 0.042 0.030
0.026 0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.040 -0.167 0.025
-0.167 0.043 -0.029
0.025 -0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.040 -0.167 -0.025
-0.167 0.042 0.029
-0.025 0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.040 0.166 -0.026
0.166 0.042 -0.030
-0.026 -0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-222.362 -17.574 -3.419
-17.574 -303.468 -44.049
-3.419 -44.049 -89.081
261.494 -4.060 -0.927
-4.060 258.056 5.856
-0.927 5.856 222.641

orbtensor 2 C
-219.822 18.349 -4.355
18.349 -305.492 43.384
-4.355 43.384 -94.639

261.477	4.036	-1.132
4.036	258.063	-5.866
-1.132	-5.866	222.651

orbtensor 3 C

-225.433	15.568	1.835
15.568	-302.935	-43.705
1.835	-43.705	-89.026
261.477	4.037	1.130
4.037	258.062	5.867
1.130	5.867	222.651

orbtensor 4 C

-221.119	-17.507	4.230
-17.507	-302.720	45.591
4.230	45.591	-88.361
261.495	-4.060	0.924
-4.060	258.056	-5.854
0.924	-5.854	222.641

orbtensor 5 C

-279.271	-8.927	1.192
-8.927	-296.354	-34.255
1.192	-34.255	-98.567
270.944	2.019	0.384
2.019	266.007	4.911
0.384	4.911	229.406

orbtensor 6 C

-281.853	9.014	1.600
9.014	-296.140	38.319
1.600	38.319	-100.112
270.956	-2.042	0.214
-2.042	266.021	-4.864
0.214	-4.864	229.412

orbtensor 7 C

-281.804	10.260	2.305
10.260	-296.000	-36.410
2.305	-36.410	-99.234
270.953	-2.041	-0.216
-2.041	266.019	4.867
-0.216	4.867	229.411

orbtensor 8 C

-282.637	-9.705	-1.646
-9.705	-295.389	36.978
-1.646	36.978	-98.897
270.944	2.019	-0.386
2.019	266.007	-4.910
-0.386	-4.910	229.405

orbtensor 9 C

-260.028	-16.678	3.762
-16.678	-257.763	-19.947
3.762	-19.947	-74.490
262.817	0.533	0.714
0.533	262.805	2.897
0.714	2.897	217.367

orbtensor 10 C

-258.075	16.776	2.631
16.776	-256.206	18.355
2.631	18.355	-74.760
262.813	-0.548	0.564
-0.548	262.836	-2.743
0.564	-2.743	217.353

orbtensor 11 C
-259.053 16.505 -2.329
16.505 -255.102 -18.427
-2.329 -18.427 -72.893
262.814 -0.548 -0.565
-0.548 262.834 2.745
-0.565 2.745 217.353

orbtensor 12 C
-259.644 -17.318 -2.280
-17.318 -256.759 21.007
-2.280 21.007 -72.020
262.815 0.535 -0.716
0.535 262.805 -2.893
-0.716 -2.893 217.365

orbtensor 13 C
-300.220 -10.661 19.115
-10.661 -283.140 -20.629
19.115 -20.629 -95.205
266.508 1.899 -0.234
1.899 271.118 1.929
-0.234 1.929 229.103

orbtensor 14 C
-299.361 9.261 21.554
9.261 -283.447 19.255
21.554 19.255 -96.204
266.514 -1.897 -0.276
-1.897 271.134 -1.751
-0.276 -1.751 229.095

orbtensor 15 C
-299.760 8.706 -19.523
8.706 -283.319 -18.030
-19.523 -18.030 -92.955
266.515 -1.898 0.276
-1.898 271.134 1.754
0.276 1.754 229.097

orbtensor 16 C
-298.786 -9.278 -19.658
-9.278 -284.538 21.670
-19.658 21.670 -91.661
266.508 1.899 0.234
1.899 271.117 -1.927
0.234 -1.927 229.102

orbtensor 17 C
-218.501 -108.469 -55.365
-108.469 -227.945 45.796
-55.365 45.796 -222.958
252.344 14.870 10.140
14.870 254.107 -8.811
10.140 -8.811 250.685

orbtensor 18 C
-218.900 107.498 -56.534
107.498 -227.150 -48.087
-56.534 -48.087 -221.677
252.384 -14.898 10.055
-14.898 254.036 8.849
10.055 8.849 250.744

orbtensor 19 C
-218.219 106.533 56.357

106.533	-228.161	46.389
56.357	46.389	-222.751
252.389	-14.894	-10.058
-14.894	254.040	-8.853
-10.058	-8.853	250.737

orbtensor 20 C

-218.946	-108.296	56.214
-108.296	-227.903	-47.905
56.214	-47.905	-224.610
252.347	14.866	-10.142
14.866	254.113	8.812
-10.142	8.812	250.685

orbtensor 23 C

-193.282	69.991	87.172
69.991	-174.808	46.914
87.172	46.914	-267.542
245.744	-15.658	-6.098
-15.658	250.614	-12.114
-6.098	-12.114	249.517

orbtensor 24 C

-193.222	-69.996	86.837
-69.996	-172.025	-47.389
86.837	-47.389	-271.332
245.733	15.657	-6.175
15.657	250.707	12.079
-6.175	12.079	249.419

orbtensor 25 C

-312.221	-16.100	23.996
-16.100	-225.653	13.001
23.996	13.001	-81.517
258.847	-4.032	-2.131
-4.032	261.430	1.193
-2.131	1.193	221.940

orbtensor 26 C

-308.989	15.571	25.399
15.571	-226.116	-12.374
25.399	-12.374	-80.989
258.850	4.042	-2.118
4.042	261.444	-0.981
-2.118	-0.981	221.933

orbtensor 27 C

-313.381	15.811	-26.469
15.811	-220.610	13.579
-26.469	13.579	-81.968
258.850	4.041	2.119
4.041	261.444	0.984
2.119	0.984	221.933

orbtensor 28 C

-308.357	-15.213	-25.179
-15.213	-225.153	-14.558
-25.179	-14.558	-81.711
258.848	-4.031	2.131
-4.031	261.430	-1.191
2.131	-1.191	221.940

orbtensor 29 C

-160.338	-73.027	-45.228
-73.027	-206.610	86.383
-45.228	86.383	-262.083
247.892	14.962	13.429

14.962 246.764 -5.422
13.429 -5.422 250.413

orbtensor 30 C
-165.514 73.669 -43.051
73.669 -205.408 -87.458
-43.051 -87.458 -265.541
247.934 -15.018 13.369
-15.018 246.724 5.428
13.369 5.428 250.400

orbtensor 31 C
-167.692 72.526 43.555
72.526 -206.088 85.026
43.555 85.026 -266.954
247.944 -15.014 -13.372
-15.014 246.724 -5.433
-13.372 -5.433 250.394

orbtensor 32 C
-164.600 -73.589 47.121
-73.589 -204.736 -87.419
47.121 -87.419 -264.097
247.893 14.959 -13.432
14.959 246.767 5.424
-13.432 5.424 250.410

orbtensor 33 C
-149.589 -78.558 -42.356
-78.558 -202.581 95.781
-42.356 95.781 -230.527
244.309 15.917 10.859
15.917 244.341 -8.472
10.859 -8.472 246.523

orbtensor 34 C
-149.043 78.293 -46.608
78.293 -204.735 -96.494
-46.608 -96.494 -229.922
244.325 -15.956 10.786
-15.956 244.272 8.486
10.786 8.486 246.559

orbtensor 35 C
-148.248 78.835 44.117
78.835 -199.365 96.060
44.117 96.060 -229.443
244.333 -15.953 -10.789
-15.953 244.271 -8.492
-10.789 -8.492 246.549

orbtensor 36 C
-150.734 -76.802 43.924
-76.802 -200.921 -94.823
43.924 -94.823 -230.340
244.310 15.915 -10.862
15.915 244.344 8.473
-10.862 8.473 246.519

orbtensor 37 C
-180.679 -71.813 -97.804
-71.813 -160.408 40.267
-97.804 40.267 -239.556
242.783 16.010 9.546
16.010 246.579 -9.528
9.546 -9.528 246.312

orbtensor 38 C
-183.341 74.154 -97.089
74.154 -158.605 -42.123
-97.089 -42.123 -238.887
242.808 -16.036 9.477
-16.036 246.515 9.553
9.477 9.553 246.371

orbtensor 39 C
-184.573 74.452 95.093
74.452 -159.115 43.342
95.093 43.342 -241.405
242.816 -16.033 -9.480
-16.033 246.513 -9.558
-9.480 -9.558 246.362

orbtensor 40 C
-181.629 -74.083 97.864
-74.083 -160.492 -42.200
97.864 -42.200 -240.278
242.782 16.008 -9.548
16.008 246.583 9.529
-9.548 9.529 246.307

orbtensor 41 C
-196.936 -117.847 -59.621
-117.847 -210.225 46.684
-59.621 46.684 -182.806
243.819 12.806 10.666
12.806 245.858 -10.145
10.666 -10.145 250.687

orbtensor 42 C
-199.465 117.228 -55.692
117.228 -212.766 -45.092
-55.692 -45.092 -184.811
243.843 -12.839 10.620
-12.839 245.775 10.140
10.620 10.140 250.745

orbtensor 43 C
-199.217 116.140 56.355
116.140 -210.060 45.939
56.355 45.939 -184.311
243.851 -12.835 -10.623
-12.835 245.776 -10.145
-10.623 -10.145 250.737

orbtensor 44 C
-195.774 -117.410 59.977
-117.410 -210.798 -47.139
59.977 -47.139 -182.394
243.821 12.804 -10.669
12.804 245.861 10.146
-10.669 10.146 250.684

orbtensor 47 H
-3.132 -8.254 -1.847
-8.254 -16.552 -3.152
-1.847 -3.152 -4.102
35.439 4.747 -0.170
4.747 35.614 3.098
-0.170 3.098 18.688

orbtensor 48 H
-3.225 8.325 -1.837
8.325 -16.580 3.249

-1.837	3.249	-4.359
35.436	-4.757	-0.249
-4.757	35.613	-3.062
-0.249	-3.062	18.684

orbtensor 49 H

-3.080	8.354	1.629
8.354	-16.428	-3.112
1.629	-3.112	-4.418
35.435	-4.757	0.248
-4.757	35.613	3.063
0.248	3.063	18.684

orbtensor 50 H

-3.142	-8.176	1.817
-8.176	-16.557	3.364
1.817	3.364	-4.324
35.440	4.747	0.170
4.747	35.614	-3.097
0.170	-3.097	18.688

orbtensor 51 H

-8.334	-1.466	-8.723
-1.466	-4.014	-1.782
-8.723	-1.782	-15.643
31.260	4.572	5.532
4.572	27.462	-3.734
5.532	-3.734	34.494

orbtensor 52 H

-8.488	1.578	-8.976
1.578	-3.862	2.014
-8.976	2.014	-15.525
31.262	-4.597	5.520
-4.597	27.434	3.702
5.520	3.702	34.509

orbtensor 53 H

-8.634	1.444	8.735
1.444	-3.871	-2.023
8.735	-2.023	-15.584
31.267	-4.595	-5.521
-4.595	27.434	-3.705
-5.521	-3.705	34.504

orbtensor 54 H

-8.428	-1.350	8.813
-1.350	-4.012	2.009
8.813	2.009	-15.690
31.261	4.571	-5.533
4.571	27.462	3.735
-5.533	3.735	34.492

orbtensor 55 H

-4.163	-1.396	2.952
-1.396	-9.918	9.282
2.952	9.282	-14.345
26.855	4.404	3.601
4.404	32.586	-5.339
3.601	-5.339	34.300

orbtensor 56 H

-4.020	1.385	2.885
1.385	-10.022	-9.410
2.885	-9.410	-14.435
26.872	-4.403	3.601
-4.403	32.537	5.340

3.601 5.340 34.335

orbtensor 57 H

-3.842 1.557 -2.937
1.557 -9.910 9.445
-2.937 9.445 -14.253
26.873 -4.401 -3.603
-4.401 32.539 -5.341
-3.603 -5.341 34.332

orbtensor 58 H

-4.207 -1.403 -2.964
-1.403 -10.054 -9.281
-2.964 -9.281 -14.378
26.855 4.403 -3.602
4.403 32.588 5.339
-3.602 5.339 34.299

orbtensor 59 H

-0.918 -3.151 0.573
-3.151 -9.132 8.904
0.573 8.904 -11.390
26.908 4.377 0.297
4.377 33.304 -8.823
0.297 -8.823 33.688

orbtensor 60 H

-0.979 3.142 0.597
3.142 -8.887 -8.874
0.597 -8.874 -11.734
26.901 -4.356 0.293
-4.356 33.221 8.829
0.293 8.829 33.775

orbtensor 61 H

-1.057 3.110 -0.654
3.110 -9.000 8.730
-0.654 8.730 -11.701
26.902 -4.355 -0.295
-4.355 33.223 -8.831
-0.295 -8.831 33.772

orbtensor 62 H

-0.809 -3.227 -0.592
-3.227 -9.176 -8.791
-0.592 -8.791 -11.407
26.908 4.376 -0.300
4.376 33.306 8.824
-0.300 8.824 33.686

orbtensor 63 H

-17.087 -8.540 2.464
-8.540 -3.256 1.549
2.464 1.549 -4.101
36.149 4.785 -1.310
4.785 35.224 1.178
-1.310 1.178 18.410

orbtensor 64 H

-17.014 8.543 2.394
8.543 -3.332 -1.580
2.394 -1.580 -3.846
36.157 -4.779 -1.343
-4.779 35.231 -1.090
-1.343 -1.090 18.399

orbtensor 65 H

-17.147	8.522	-2.357
8.522	-3.298	1.598
-2.357	1.598	-3.985
36.156	-4.780	1.343
-4.780	35.231	1.091
1.343	1.091	18.399

orbtensor 66 H

-17.159	-8.498	-2.368
-8.498	-3.181	-1.508
-2.368	-1.508	-3.945
36.149	4.785	1.311
4.785	35.225	-1.177
1.311	-1.177	18.410

orbtensor 67 H

-7.819	-2.326	-8.440
-2.326	-1.128	-0.024
-8.440	-0.024	-12.869
31.856	3.759	8.930
3.759	27.157	-0.500
8.930	-0.500	35.029

orbtensor 68 H

-7.795	2.296	-8.526
2.296	-1.273	0.061
-8.526	0.061	-12.834
31.890	-3.807	8.918
-3.807	27.156	0.461
8.918	0.461	34.997

orbtensor 69 H

-7.651	2.383	8.605
2.383	-1.136	-0.048
8.605	-0.048	-12.822
31.895	-3.806	-8.919
-3.806	27.155	-0.464
-8.919	-0.464	34.992

orbtensor 70 H

-7.761	-2.262	8.613
-2.262	-1.043	-0.093
8.613	-0.093	-12.842
31.857	3.759	-8.930
3.759	27.157	0.500
-8.930	0.500	35.027

orbtensor 71 H

-8.530	-11.264	-2.022
-11.264	-9.069	0.635
-2.022	0.635	-1.664
33.478	9.739	2.336
9.739	34.041	-1.085
2.336	-1.085	26.825

orbtensor 72 H

-8.676	11.200	-1.929
11.200	-9.325	-0.713
-1.929	-0.713	-1.923
33.472	-9.749	2.272
-9.749	34.047	1.140
2.272	1.140	26.827

orbtensor 73 H

-8.531	11.162	1.862
11.162	-9.259	0.704
1.862	0.704	-1.917

33.475 -9.748 -2.272
 -9.748 34.044 -1.142
 -2.272 -1.142 26.826

orbtensor 74 H
 -8.344 -11.343 2.094
 -11.343 -8.976 -0.657
 2.094 -0.657 -1.669
 33.477 9.738 -2.336
 9.738 34.043 1.085
 -2.336 1.085 26.825

gtensor (ppt)
 -0.151 0.000 0.000
 0.000 -0.156 0.000
 0.000 0.000 -0.239
 38.654 -1.060 -1.414
 -1.060 40.681 -2.586
 -1.414 -2.586 17.581

zfstensor (cm-1)
 2.389903 -0.007870 0.003689
 -0.007870 1.548798 -0.005294
 0.003689 -0.005294 125.987003

averaging
 A Average:5,6,7,8,13,14,15,16
 B Average:1,2,3,4,25,26,27,28
 M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4067	42.42667	205.69997	9.91391	215.61387	258.04054
2	C	-0.4097	40.74600	207.21743	9.62661	216.84404	257.59004
3	C	-0.4097	41.59867	207.21743	9.85778	217.07520	258.67387
4	C	-0.4067	43.33067	205.69997	9.70322	215.40319	258.73386
5	C	-1.1003	30.72167	556.57016	-31.54519	525.02497	555.74663
6	C	-1.0967	29.42800	554.71548	-32.40445	522.31103	551.73903
7	C	-1.0967	29.78167	554.71548	-32.10230	522.61318	552.39485
8	C	-1.1003	29.81100	556.57016	-32.05078	524.51938	554.33038
9	C	0.4347	50.23600	-219.86292	-1.30809	-221.17101	-170.93501
10	C	0.4333	51.32033	-219.18849	-1.82820	-221.01669	-169.69635
11	C	0.4337	51.98433	-219.35710	-1.91285	-221.26995	-169.28561
12	C	0.4347	51.52067	-219.86292	-1.45962	-221.32254	-169.80187
13	C	-0.9447	29.38800	477.83091	-37.97796	439.85294	469.24094
14	C	-0.9433	29.24367	477.15648	-38.43164	438.72484	467.96851
15	C	-0.9433	30.23733	477.15648	-38.50909	438.64739	468.88472
16	C	-0.9447	30.58067	477.83091	-38.30029	439.53062	470.11129
17	C	-0.0983	29.24400	49.73893	-14.30462	35.43431	64.67831
18	C	-0.0980	29.81233	49.57032	-14.45769	35.11263	64.92496
19	C	-0.0980	29.34500	49.57032	-14.45771	35.11261	64.45761
20	C	-0.0983	28.56200	49.73893	-14.36023	35.37869	63.94069
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1587	36.74767	-80.25671	-11.38373	-91.64044	-54.89277
24	C	0.1587	36.42667	-80.25671	-11.32882	-91.58553	-55.15886
25	C	-0.3323	40.94200	168.10071	-5.10427	162.99644	203.93844
26	C	-0.3307	42.04433	167.25768	-5.21090	162.04678	204.09111
27	C	-0.3303	42.08933	167.08907	-5.39261	161.69646	203.78579
28	C	-0.3323	42.33233	168.10071	-5.20820	162.89251	205.22484
29	C	0.1403	38.67933	-70.98335	-7.60024	-78.58358	-39.90425
30	C	0.1403	36.19833	-70.98335	-7.78895	-78.77230	-42.57397
31	C	0.1403	34.77600	-70.98335	-7.77104	-78.75439	-43.97839
32	C	0.1403	37.21233	-70.98335	-7.66910	-78.65245	-41.44012
33	C	-0.0010	50.82533	0.50582	-5.31307	-4.80725	46.01809

34	C	-0.0007	50.48533	0.33721	-5.27433	-4.93712	45.54821
35	C	-0.0010	52.69900	0.50582	-5.35023	-4.84441	47.85459
36	C	-0.0010	51.05933	0.50582	-5.30919	-4.80337	46.25596
A Average		-1.0212	29.89900	516.56826	-35.16521	481.40304	511.30204
B Average		-0.3698	41.93875	187.04787	2.27319	189.32106	231.25981
M Average		0.4341	51.26533	-219.56785	-1.62719	-221.19504	-169.92971

=====

FeL5-planar-LS-STO-PBE0-No-ZFS

Temperature: 303

Spin: 1.5

atensor 1 C

-0.611 0.169 -0.023
0.169 -0.279 0.292
-0.023 0.292 -0.308
-0.031 -0.003 -0.001
0.007 0.010 0.002
-0.002 0.001 -0.001

atensor 2 C

-0.614 -0.170 -0.021
-0.170 -0.282 -0.292
-0.021 -0.292 -0.311
-0.031 0.003 -0.001
-0.007 0.010 -0.002
-0.002 -0.001 -0.001

atensor 3 C

-0.614 -0.170 0.021
-0.170 -0.282 0.292
0.021 0.292 -0.311
-0.031 0.003 0.001
-0.007 0.010 0.002
0.002 0.001 -0.001

atensor 4 C

-0.611 0.169 0.023
0.169 -0.279 -0.292
0.023 -0.292 -0.308
-0.031 -0.003 0.001
0.007 0.010 -0.002
0.002 -0.001 -0.001

atensor 5 C

-1.430 0.447 0.228
0.447 -0.451 0.534
0.228 0.534 -1.407
-0.013 0.014 0.007
0.034 0.000 0.006
0.005 0.000 0.000

atensor 6 C

-1.425 -0.450 0.229
-0.450 -0.446 -0.533
0.229 -0.533 -1.406
-0.013 -0.014 0.007
-0.034 0.000 -0.006
0.005 0.000 0.000

atensor 7 C

-1.425 -0.450 -0.229
-0.450 -0.446 0.533
-0.229 0.533 -1.406
-0.013 -0.014 -0.007
-0.034 0.000 0.006

-0.005 0.000 0.000

atensor 8 C

-1.430 0.447 -0.228
0.447 -0.451 -0.534
-0.228 -0.534 -1.407
-0.013 0.014 -0.007
0.034 0.000 -0.006
-0.005 0.000 0.000

atensor 9 C

0.429 0.641 0.348
0.641 0.449 -0.002
0.348 -0.002 0.422
0.004 0.008 0.002
0.002 0.002 0.002
0.004 0.001 -0.002

atensor 10 C

0.431 -0.643 0.348
-0.643 0.447 0.003
0.348 0.003 0.419
0.004 -0.008 0.002
-0.002 0.002 -0.002
0.004 -0.002 -0.003

atensor 11 C

0.431 -0.643 -0.348
-0.643 0.447 -0.003
-0.348 -0.003 0.420
0.004 -0.008 -0.002
-0.002 0.002 0.002
-0.004 0.002 -0.003

atensor 12 C

0.429 0.641 -0.348
0.641 0.449 0.002
-0.348 0.002 0.422
0.004 0.008 -0.002
0.002 0.002 -0.002
-0.004 -0.001 -0.002

atensor 13 C

-0.188 0.489 0.459
0.489 -1.320 0.161
0.459 0.161 -1.324
0.006 0.029 0.008
0.011 -0.007 0.004
0.001 -0.001 -0.001

atensor 14 C

-0.184 -0.490 0.457
-0.490 -1.320 -0.161
0.457 -0.161 -1.324
0.006 -0.029 0.008
-0.011 -0.007 -0.004
0.001 0.001 -0.001

atensor 15 C

-0.184 -0.490 -0.458
-0.490 -1.320 0.161
-0.458 0.161 -1.324
0.006 -0.029 -0.008
-0.011 -0.007 0.004
-0.001 -0.001 -0.001

atensor 16 C

-0.188 0.489 -0.459
0.489 -1.320 -0.161
-0.459 -0.161 -1.324
0.006 0.029 -0.008
0.011 -0.007 -0.004
-0.001 0.000 -0.001

atensor 17 C
-0.032 0.233 0.063
0.233 -0.028 0.037
0.063 0.037 -0.238
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.001

atensor 18 C
-0.031 -0.233 0.061
-0.233 -0.028 -0.036
0.062 -0.036 -0.238
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.001

atensor 19 C
-0.031 -0.233 -0.062
-0.233 -0.028 0.036
-0.062 0.036 -0.238
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 20 C
-0.032 0.233 -0.063
0.233 -0.028 -0.037
-0.063 -0.037 -0.238
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 23 C
0.170 -0.137 0.013
-0.137 0.256 -0.002
0.013 -0.002 0.049
0.000 -0.003 0.000
-0.003 0.002 0.000
0.000 0.000 -0.001

atensor 24 C
0.170 0.136 0.012
0.136 0.256 0.001
0.012 0.001 0.049
0.000 0.003 0.000
0.003 0.002 0.000
0.000 0.000 -0.001

atensor 25 C
-0.046 0.157 0.290
0.157 -0.545 -0.031
0.290 -0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 0.001
0.002 0.002 -0.001

atensor 26 C
-0.043 -0.158 0.290
-0.158 -0.544 0.031
0.290 0.031 -0.384

0.010 -0.007 0.000
0.003 -0.030 -0.001
0.002 -0.002 -0.001

atensor 27 C
-0.042 -0.158 -0.290
-0.158 -0.544 -0.031
-0.290 -0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 0.001
-0.002 0.002 -0.001

atensor 28 C
-0.046 0.157 -0.290
0.157 -0.545 0.031
-0.290 0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 -0.001
-0.002 -0.002 -0.001

atensor 29 C
0.216 0.108 0.057
0.108 0.139 0.057
0.057 0.057 0.066
0.001 0.002 0.001
0.002 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.216 -0.108 0.057
-0.108 0.140 -0.056
0.057 -0.056 0.065
0.001 -0.002 0.001
-0.002 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.216 -0.108 -0.057
-0.108 0.140 0.056
-0.057 0.056 0.065
0.001 -0.002 -0.001
-0.002 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.216 0.108 -0.057
0.108 0.139 -0.057
-0.057 -0.057 0.066
0.001 0.002 -0.001
0.002 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.012 0.089 0.005
0.089 0.037 -0.008
0.005 -0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 34 C
0.012 -0.089 0.004
-0.089 0.037 0.008
0.004 0.008 -0.052
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 35 C
0.012 -0.089 -0.004
-0.089 0.037 -0.008
-0.004 -0.008 -0.053
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 36 C
0.012 0.089 -0.005
0.089 0.037 0.008
-0.005 0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 37 C
0.025 0.078 0.036
0.078 0.009 0.020
0.036 0.020 -0.039
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.025 -0.078 0.036
-0.078 0.009 -0.020
0.036 -0.020 -0.039
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.025 -0.078 -0.036
-0.078 0.009 0.020
-0.036 0.020 -0.039
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.025 0.078 -0.036
0.078 0.009 -0.020
-0.036 -0.020 -0.039
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.039 0.045 -0.001
0.045 0.037 0.022
-0.001 0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.039 -0.046 -0.002
-0.046 0.037 -0.021
-0.002 -0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.039 -0.046 0.002

-0.046 0.037 0.021
0.002 0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.039 0.045 0.001
0.045 0.037 -0.022
0.001 -0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.608 0.359 0.031
0.359 0.644 0.299
0.031 0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 0.006
0.000 0.002 -0.004

atensor 48 H
-0.608 -0.360 0.031
-0.360 0.645 -0.297
0.031 -0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 -0.005
0.000 -0.002 -0.004

atensor 49 H
-0.607 -0.360 -0.031
-0.360 0.645 0.297
-0.031 0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 0.005
0.000 0.002 -0.004

atensor 50 H
-0.608 0.359 -0.031
0.359 0.644 -0.299
-0.031 -0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 -0.006
0.000 -0.002 -0.004

atensor 51 H
-0.065 0.641 -0.138
0.641 0.451 -0.222
-0.138 -0.222 -0.426
-0.001 0.012 -0.003
0.012 0.009 -0.004
-0.001 -0.002 -0.004

atensor 52 H
-0.065 -0.643 -0.142
-0.643 0.451 0.227
-0.142 0.227 -0.426
-0.001 -0.012 -0.003
-0.012 0.009 0.004
-0.002 0.002 -0.004

atensor 53 H
-0.065 -0.643 0.141
-0.643 0.451 -0.227
0.141 -0.227 -0.426
-0.001 -0.012 0.003

-0.012 0.009 -0.004
0.002 -0.002 -0.004

atensor 54 H
-0.065 0.641 0.138
0.641 0.451 0.222
0.138 0.222 -0.426
-0.001 0.012 0.003
0.012 0.009 0.004
0.001 0.002 -0.004

atensor 55 H
0.237 0.433 0.408
0.433 -0.123 0.260
0.408 0.260 -0.155
0.005 0.009 0.008
0.009 -0.002 0.005
0.004 0.002 -0.001

atensor 56 H
0.238 -0.434 0.405
-0.434 -0.121 -0.259
0.405 -0.259 -0.158
0.005 -0.009 0.008
-0.009 -0.002 -0.005
0.004 -0.002 -0.001

atensor 57 H
0.238 -0.434 -0.405
-0.434 -0.121 0.259
-0.405 0.259 -0.158
0.005 -0.009 -0.008
-0.009 -0.002 0.005
-0.004 0.002 -0.001

atensor 58 H
0.237 0.433 -0.408
0.433 -0.123 -0.260
-0.408 -0.260 -0.155
0.005 0.009 -0.008
0.009 -0.002 -0.005
-0.004 -0.002 -0.001

atensor 59 H
0.026 0.235 -0.031
0.235 0.151 -0.042
-0.031 -0.042 -0.143
0.000 0.004 -0.001
0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 60 H
0.026 -0.235 -0.032
-0.235 0.151 0.044
-0.032 0.044 -0.143
0.000 -0.004 -0.001
-0.004 0.003 0.001
0.000 0.000 -0.001

atensor 61 H
0.026 -0.235 0.032
-0.235 0.151 -0.044
0.032 -0.044 -0.143
0.000 -0.004 0.001
-0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 62 H
0.026 0.235 0.031
0.235 0.151 0.042
0.031 0.042 -0.143
0.000 0.004 0.001
0.004 0.003 0.001
0.000 0.000 -0.001

atensor 63 H
0.730 0.370 0.145
0.370 -0.621 -0.001
0.145 -0.001 -0.623
0.018 0.008 0.002
0.003 -0.013 0.001
0.001 0.001 -0.005

atensor 64 H
0.733 -0.370 0.143
-0.370 -0.620 0.002
0.143 0.002 -0.622
0.018 -0.008 0.002
-0.003 -0.013 -0.001
0.001 -0.001 -0.005

atensor 65 H
0.733 -0.370 -0.143
-0.370 -0.620 -0.002
-0.143 -0.002 -0.622
0.018 -0.008 -0.002
-0.003 -0.013 0.001
-0.001 0.001 -0.005

atensor 66 H
0.730 0.370 -0.145
0.370 -0.621 0.001
-0.145 0.001 -0.623
0.018 0.008 -0.002
0.003 -0.013 -0.001
-0.001 -0.001 -0.005

atensor 67 H
0.106 0.189 0.114
0.189 0.007 0.087
0.114 0.087 -0.083
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.106 -0.190 0.113
-0.190 0.008 -0.086
0.113 -0.086 -0.084
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.106 -0.190 -0.113
-0.190 0.008 0.086
-0.113 0.086 -0.084
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.106 0.189 -0.114
0.189 0.007 -0.087

-0.114 -0.087 -0.083
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.040 0.166 0.026
0.166 0.042 0.030
0.026 0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.040 -0.167 0.025
-0.167 0.043 -0.029
0.025 -0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.040 -0.167 -0.025
-0.167 0.042 0.029
-0.025 0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.040 0.166 -0.026
0.166 0.042 -0.030
-0.026 -0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-222.362 -17.574 -3.419
-17.574 -303.468 -44.049
-3.419 -44.049 -89.081
261.494 -4.060 -0.927
-4.060 258.056 5.856
-0.927 5.856 222.641

orbtensor 2 C
-219.822 18.349 -4.355
18.349 -305.492 43.384
-4.355 43.384 -94.639
261.477 4.036 -1.132
4.036 258.063 -5.866
-1.132 -5.866 222.651

orbtensor 3 C
-225.433 15.568 1.835
15.568 -302.935 -43.705
1.835 -43.705 -89.026
261.477 4.037 1.130
4.037 258.062 5.867
1.130 5.867 222.651

orbtensor 4 C
-221.119 -17.507 4.230
-17.507 -302.720 45.591
4.230 45.591 -88.361
261.495 -4.060 0.924
-4.060 258.056 -5.854


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0.924    -5.854    222.641

orbtensor 5 C
-279.271    -8.927     1.192
-8.927   -296.354   -34.255
1.192   -34.255   -98.567
270.944     2.019     0.384
2.019   266.007     4.911
0.384     4.911   229.406

orbtensor 6 C
-281.853     9.014     1.600
9.014  -296.140    38.319
1.600   38.319  -100.112
270.956    -2.042     0.214
-2.042  266.021    -4.864
0.214   -4.864   229.412

orbtensor 7 C
-281.804    10.260     2.305
10.260  -296.000   -36.410
2.305   -36.410  -99.234
270.953    -2.041    -0.216
-2.041  266.019     4.867
-0.216     4.867   229.411

orbtensor 8 C
-282.637    -9.705    -1.646
-9.705  -295.389    36.978
-1.646   36.978  -98.897
270.944     2.019    -0.386
2.019   266.007    -4.910
-0.386   -4.910   229.405

orbtensor 9 C
-260.028   -16.678     3.762
-16.678  -257.763   -19.947
3.762   -19.947  -74.490
262.817     0.533     0.714
0.533   262.805     2.897
0.714     2.897   217.367

orbtensor 10 C
-258.075    16.776     2.631
16.776  -256.206    18.355
2.631   18.355   -74.760
262.813    -0.548     0.564
-0.548  262.836    -2.743
0.564   -2.743   217.353

orbtensor 11 C
-259.053    16.505    -2.329
16.505  -255.102   -18.427
-2.329  -18.427   -72.893
262.814    -0.548    -0.565
-0.548  262.834     2.745
-0.565     2.745   217.353

orbtensor 12 C
-259.644   -17.318    -2.280
-17.318  -256.759    21.007
-2.280   21.007   -72.020
262.815     0.535    -0.716
0.535   262.805    -2.893
-0.716   -2.893   217.365

orbtensor 13 C

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-300.220	-10.661	19.115
-10.661	-283.140	-20.629
19.115	-20.629	-95.205
266.508	1.899	-0.234
1.899	271.118	1.929
-0.234	1.929	229.103

orbtensor 14 C

-299.361	9.261	21.554
9.261	-283.447	19.255
21.554	19.255	-96.204
266.514	-1.897	-0.276
-1.897	271.134	-1.751
-0.276	-1.751	229.095

orbtensor 15 C

-299.760	8.706	-19.523
8.706	-283.319	-18.030
-19.523	-18.030	-92.955
266.515	-1.898	0.276
-1.898	271.134	1.754
0.276	1.754	229.097

orbtensor 16 C

-298.786	-9.278	-19.658
-9.278	-284.538	21.670
-19.658	21.670	-91.661
266.508	1.899	0.234
1.899	271.117	-1.927
0.234	-1.927	229.102

orbtensor 17 C

-218.501	-108.469	-55.365
-108.469	-227.945	45.796
-55.365	45.796	-222.958
252.344	14.870	10.140
14.870	254.107	-8.811
10.140	-8.811	250.685

orbtensor 18 C

-218.900	107.498	-56.534
107.498	-227.150	-48.087
-56.534	-48.087	-221.677
252.384	-14.898	10.055
-14.898	254.036	8.849
10.055	8.849	250.744

orbtensor 19 C

-218.219	106.533	56.357
106.533	-228.161	46.389
56.357	46.389	-222.751
252.389	-14.894	-10.058
-14.894	254.040	-8.853
-10.058	-8.853	250.737

orbtensor 20 C

-218.946	-108.296	56.214
-108.296	-227.903	-47.905
56.214	-47.905	-224.610
252.347	14.866	-10.142
14.866	254.113	8.812
-10.142	8.812	250.685

orbtensor 23 C

-193.282	69.991	87.172
69.991	-174.808	46.914
87.172	46.914	-267.542

245.744 -15.658 -6.098
-15.658 250.614 -12.114
-6.098 -12.114 249.517

orbtensor 24 C
-193.222 -69.996 86.837
-69.996 -172.025 -47.389
86.837 -47.389 -271.332
245.733 15.657 -6.175
15.657 250.707 12.079
-6.175 12.079 249.419

orbtensor 25 C
-312.221 -16.100 23.996
-16.100 -225.653 13.001
23.996 13.001 -81.517
258.847 -4.032 -2.131
-4.032 261.430 1.193
-2.131 1.193 221.940

orbtensor 26 C
-308.989 15.571 25.399
15.571 -226.116 -12.374
25.399 -12.374 -80.989
258.850 4.042 -2.118
4.042 261.444 -0.981
-2.118 -0.981 221.933

orbtensor 27 C
-313.381 15.811 -26.469
15.811 -220.610 13.579
-26.469 13.579 -81.968
258.850 4.041 2.119
4.041 261.444 0.984
2.119 0.984 221.933

orbtensor 28 C
-308.357 -15.213 -25.179
-15.213 -225.153 -14.558
-25.179 -14.558 -81.711
258.848 -4.031 2.131
-4.031 261.430 -1.191
2.131 -1.191 221.940

orbtensor 29 C
-160.338 -73.027 -45.228
-73.027 -206.610 86.383
-45.228 86.383 -262.083
247.892 14.962 13.429
14.962 246.764 -5.422
13.429 -5.422 250.413

orbtensor 30 C
-165.514 73.669 -43.051
73.669 -205.408 -87.458
-43.051 -87.458 -265.541
247.934 -15.018 13.369
-15.018 246.724 5.428
13.369 5.428 250.400

orbtensor 31 C
-167.692 72.526 43.555
72.526 -206.088 85.026
43.555 85.026 -266.954
247.944 -15.014 -13.372
-15.014 246.724 -5.433
-13.372 -5.433 250.394

orbtensor 32 C
-164.600 -73.589 47.121
-73.589 -204.736 -87.419
47.121 -87.419 -264.097
247.893 14.959 -13.432
14.959 246.767 5.424
-13.432 5.424 250.410

orbtensor 33 C
-149.589 -78.558 -42.356
-78.558 -202.581 95.781
-42.356 95.781 -230.527
244.309 15.917 10.859
15.917 244.341 -8.472
10.859 -8.472 246.523

orbtensor 34 C
-149.043 78.293 -46.608
78.293 -204.735 -96.494
-46.608 -96.494 -229.922
244.325 -15.956 10.786
-15.956 244.272 8.486
10.786 8.486 246.559

orbtensor 35 C
-148.248 78.835 44.117
78.835 -199.365 96.060
44.117 96.060 -229.443
244.333 -15.953 -10.789
-15.953 244.271 -8.492
-10.789 -8.492 246.549

orbtensor 36 C
-150.734 -76.802 43.924
-76.802 -200.921 -94.823
43.924 -94.823 -230.340
244.310 15.915 -10.862
15.915 244.344 8.473
-10.862 8.473 246.519

orbtensor 37 C
-180.679 -71.813 -97.804
-71.813 -160.408 40.267
-97.804 40.267 -239.556
242.783 16.010 9.546
16.010 246.579 -9.528
9.546 -9.528 246.312

orbtensor 38 C
-183.341 74.154 -97.089
74.154 -158.605 -42.123
-97.089 -42.123 -238.887
242.808 -16.036 9.477
-16.036 246.515 9.553
9.477 9.553 246.371

orbtensor 39 C
-184.573 74.452 95.093
74.452 -159.115 43.342
95.093 43.342 -241.405
242.816 -16.033 -9.480
-16.033 246.513 -9.558
-9.480 -9.558 246.362

orbtensor 40 C
-181.629 -74.083 97.864

-74.083	-160.492	-42.200
97.864	-42.200	-240.278
242.782	16.008	-9.548
16.008	246.583	9.529
-9.548	9.529	246.307

orbtensor 41 C

-196.936	-117.847	-59.621
-117.847	-210.225	46.684
-59.621	46.684	-182.806
243.819	12.806	10.666
12.806	245.858	-10.145
10.666	-10.145	250.687

orbtensor 42 C

-199.465	117.228	-55.692
117.228	-212.766	-45.092
-55.692	-45.092	-184.811
243.843	-12.839	10.620
-12.839	245.775	10.140
10.620	10.140	250.745

orbtensor 43 C

-199.217	116.140	56.355
116.140	-210.060	45.939
56.355	45.939	-184.311
243.851	-12.835	-10.623
-12.835	245.776	-10.145
-10.623	-10.145	250.737

orbtensor 44 C

-195.774	-117.410	59.977
-117.410	-210.798	-47.139
59.977	-47.139	-182.394
243.821	12.804	-10.669
12.804	245.861	10.146
-10.669	10.146	250.684

orbtensor 47 H

-3.132	-8.254	-1.847
-8.254	-16.552	-3.152
-1.847	-3.152	-4.102
35.439	4.747	-0.170
4.747	35.614	3.098
-0.170	3.098	18.688

orbtensor 48 H

-3.225	8.325	-1.837
8.325	-16.580	3.249
-1.837	3.249	-4.359
35.436	-4.757	-0.249
-4.757	35.613	-3.062
-0.249	-3.062	18.684

orbtensor 49 H

-3.080	8.354	1.629
8.354	-16.428	-3.112
1.629	-3.112	-4.418
35.435	-4.757	0.248
-4.757	35.613	3.063
0.248	3.063	18.684

orbtensor 50 H

-3.142	-8.176	1.817
-8.176	-16.557	3.364
1.817	3.364	-4.324
35.440	4.747	0.170

4.747 35.614 -3.097
0.170 -3.097 18.688

orbtensor 51 H
-8.334 -1.466 -8.723
-1.466 -4.014 -1.782
-8.723 -1.782 -15.643
31.260 4.572 5.532
4.572 27.462 -3.734
5.532 -3.734 34.494

orbtensor 52 H
-8.488 1.578 -8.976
1.578 -3.862 2.014
-8.976 2.014 -15.525
31.262 -4.597 5.520
-4.597 27.434 3.702
5.520 3.702 34.509

orbtensor 53 H
-8.634 1.444 8.735
1.444 -3.871 -2.023
8.735 -2.023 -15.584
31.267 -4.595 -5.521
-4.595 27.434 -3.705
-5.521 -3.705 34.504

orbtensor 54 H
-8.428 -1.350 8.813
-1.350 -4.012 2.009
8.813 2.009 -15.690
31.261 4.571 -5.533
4.571 27.462 3.735
-5.533 3.735 34.492

orbtensor 55 H
-4.163 -1.396 2.952
-1.396 -9.918 9.282
2.952 9.282 -14.345
26.855 4.404 3.601
4.404 32.586 -5.339
3.601 -5.339 34.300

orbtensor 56 H
-4.020 1.385 2.885
1.385 -10.022 -9.410
2.885 -9.410 -14.435
26.872 -4.403 3.601
-4.403 32.537 5.340
3.601 5.340 34.335

orbtensor 57 H
-3.842 1.557 -2.937
1.557 -9.910 9.445
-2.937 9.445 -14.253
26.873 -4.401 -3.603
-4.401 32.539 -5.341
-3.603 -5.341 34.332

orbtensor 58 H
-4.207 -1.403 -2.964
-1.403 -10.054 -9.281
-2.964 -9.281 -14.378
26.855 4.403 -3.602
4.403 32.588 5.339
-3.602 5.339 34.299

orbtensor 59 H
-0.918 -3.151 0.573
-3.151 -9.132 8.904
0.573 8.904 -11.390
26.908 4.377 0.297
4.377 33.304 -8.823
0.297 -8.823 33.688

orbtensor 60 H
-0.979 3.142 0.597
3.142 -8.887 -8.874
0.597 -8.874 -11.734
26.901 -4.356 0.293
-4.356 33.221 8.829
0.293 8.829 33.775

orbtensor 61 H
-1.057 3.110 -0.654
3.110 -9.000 8.730
-0.654 8.730 -11.701
26.902 -4.355 -0.295
-4.355 33.223 -8.831
-0.295 -8.831 33.772

orbtensor 62 H
-0.809 -3.227 -0.592
-3.227 -9.176 -8.791
-0.592 -8.791 -11.407
26.908 4.376 -0.300
4.376 33.306 8.824
-0.300 8.824 33.686

orbtensor 63 H
-17.087 -8.540 2.464
-8.540 -3.256 1.549
2.464 1.549 -4.101
36.149 4.785 -1.310
4.785 35.224 1.178
-1.310 1.178 18.410

orbtensor 64 H
-17.014 8.543 2.394
8.543 -3.332 -1.580
2.394 -1.580 -3.846
36.157 -4.779 -1.343
-4.779 35.231 -1.090
-1.343 -1.090 18.399

orbtensor 65 H
-17.147 8.522 -2.357
8.522 -3.298 1.598
-2.357 1.598 -3.985
36.156 -4.780 1.343
-4.780 35.231 1.091
1.343 1.091 18.399

orbtensor 66 H
-17.159 -8.498 -2.368
-8.498 -3.181 -1.508
-2.368 -1.508 -3.945
36.149 4.785 1.311
4.785 35.225 -1.177
1.311 -1.177 18.410

orbtensor 67 H
-7.819 -2.326 -8.440
-2.326 -1.128 -0.024

-8.440	-0.024	-12.869
31.856	3.759	8.930
3.759	27.157	-0.500
8.930	-0.500	35.029

orbtensor 68 H

-7.795	2.296	-8.526
2.296	-1.273	0.061
-8.526	0.061	-12.834
31.890	-3.807	8.918
-3.807	27.156	0.461
8.918	0.461	34.997

orbtensor 69 H

-7.651	2.383	8.605
2.383	-1.136	-0.048
8.605	-0.048	-12.822
31.895	-3.806	-8.919
-3.806	27.155	-0.464
-8.919	-0.464	34.992

orbtensor 70 H

-7.761	-2.262	8.613
-2.262	-1.043	-0.093
8.613	-0.093	-12.842
31.857	3.759	-8.930
3.759	27.157	0.500
-8.930	0.500	35.027

orbtensor 71 H

-8.530	-11.264	-2.022
-11.264	-9.069	0.635
-2.022	0.635	-1.664
33.478	9.739	2.336
9.739	34.041	-1.085
2.336	-1.085	26.825

orbtensor 72 H

-8.676	11.200	-1.929
11.200	-9.325	-0.713
-1.929	-0.713	-1.923
33.472	-9.749	2.272
-9.749	34.047	1.140
2.272	1.140	26.827

orbtensor 73 H

-8.531	11.162	1.862
11.162	-9.259	0.704
1.862	0.704	-1.917
33.475	-9.748	-2.272
-9.748	34.044	-1.142
-2.272	-1.142	26.826

orbtensor 74 H

-8.344	-11.343	2.094
-11.343	-8.976	-0.657
2.094	-0.657	-1.669
33.477	9.738	-2.336
9.738	34.043	1.085
-2.336	1.085	26.825

gtensor (ppt)

-0.151	0.000	0.000
0.000	-0.156	0.000
0.000	0.000	-0.239
38.654	-1.060	-1.414
-1.060	40.681	-2.586

-1.414 -2.586 17.581

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4067	42.42667	214.09784	0.31050	214.40834	256.83501
2	C	-0.4097	40.74600	215.67725	-0.01362	215.66363	256.40963
3	C	-0.4097	41.59867	215.67725	0.25924	215.93649	257.53516
4	C	-0.4067	43.33067	214.09784	0.06057	214.15841	257.48908
5	C	-1.1003	30.72167	579.29260	-0.29024	579.00237	609.72403
6	C	-1.0967	29.42800	577.36221	-0.94661	576.41561	605.84361
7	C	-1.0967	29.78167	577.36221	-0.58300	576.77921	606.56088
8	C	-1.1003	29.81100	579.29260	-0.88355	578.40905	608.22005
9	C	0.4347	50.23600	-228.83900	0.17391	-228.66509	-178.42909
10	C	0.4333	51.32033	-228.13704	-0.06680	-228.20385	-176.88351
11	C	0.4337	51.98433	-228.31253	-0.23767	-228.55020	-176.56587
12	C	0.4347	51.52067	-228.83900	0.00311	-228.83589	-177.31522
13	C	-0.9447	29.38800	497.33876	-0.34891	496.98985	526.37785
14	C	-0.9433	29.24367	496.63680	-0.68293	495.95386	525.19753
15	C	-0.9433	30.23733	496.63680	-0.76334	495.87345	526.11079
16	C	-0.9447	30.58067	497.33876	-0.72026	496.61850	527.19917
17	C	-0.0983	29.24400	51.76956	-0.19392	51.57564	80.81964
18	C	-0.0980	29.81233	51.59407	-0.31409	51.27998	81.09232
19	C	-0.0980	29.34500	51.59407	-0.31258	51.28149	80.62649
20	C	-0.0983	28.56200	51.76956	-0.25816	51.51140	80.07340
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1587	36.74767	-83.53326	-0.24265	-83.77591	-47.02824
24	C	0.1587	36.42667	-83.53326	-0.19054	-83.72379	-47.29713
25	C	-0.3323	40.94200	174.96356	0.03127	174.99483	215.93683
26	C	-0.3307	42.04433	174.08611	-0.00185	174.08427	216.12860
27	C	-0.3303	42.08933	173.91062	-0.17069	173.73993	215.82926
28	C	-0.3323	42.33233	174.96356	-0.08438	174.87918	217.21151
29	C	0.1403	38.67933	-73.88130	-0.07714	-73.95844	-35.27911
30	C	0.1403	36.19833	-73.88130	-0.17067	-74.05198	-37.85364
31	C	0.1403	34.77600	-73.88130	-0.14811	-74.02942	-39.25342
32	C	0.1403	37.21233	-73.88130	-0.15718	-74.03849	-36.82616
33	C	-0.0010	50.82533	0.52647	-0.08743	0.43904	51.26438
34	C	-0.0007	50.48533	0.35098	-0.11254	0.23844	50.72377
35	C	-0.0010	52.69900	0.52647	-0.12291	0.40356	53.10256
36	C	-0.0010	51.05933	0.52647	-0.08273	0.44374	51.50307
A Average		-1.0212	29.89900	537.65759	-0.65235	537.00524	566.90424
B Average		-0.3698	41.93875	194.68426	0.04888	194.73314	236.67189
M Average		0.4341	51.26533	-228.53190	-0.03186	-228.56376	-177.29842

=====
FeL5-planar-LS-STO-PBE0-No-G

Temperature: 303

Spin: 1.5

atensor 1 C

-0.611 0.169 -0.023

0.169 -0.279 0.292

-0.023 0.292 -0.308

-0.031 -0.003 -0.001

0.007 0.010 0.002

-0.002 0.001 -0.001

atensor 2 C

-0.614 -0.170 -0.021

-0.170 -0.282 -0.292
-0.021 -0.292 -0.311
-0.031 0.003 -0.001
-0.007 0.010 -0.002
-0.002 -0.001 -0.001

atensor 3 C
-0.614 -0.170 0.021
-0.170 -0.282 0.292
0.021 0.292 -0.311
-0.031 0.003 0.001
-0.007 0.010 0.002
0.002 0.001 -0.001

atensor 4 C
-0.611 0.169 0.023
0.169 -0.279 -0.292
0.023 -0.292 -0.308
-0.031 -0.003 0.001
0.007 0.010 -0.002
0.002 -0.001 -0.001

atensor 5 C
-1.430 0.447 0.228
0.447 -0.451 0.534
0.228 0.534 -1.407
-0.013 0.014 0.007
0.034 0.000 0.006
0.005 0.000 0.000

atensor 6 C
-1.425 -0.450 0.229
-0.450 -0.446 -0.533
0.229 -0.533 -1.406
-0.013 -0.014 0.007
-0.034 0.000 -0.006
0.005 0.000 0.000

atensor 7 C
-1.425 -0.450 -0.229
-0.450 -0.446 0.533
-0.229 0.533 -1.406
-0.013 -0.014 -0.007
-0.034 0.000 0.006
-0.005 0.000 0.000

atensor 8 C
-1.430 0.447 -0.228
0.447 -0.451 -0.534
-0.228 -0.534 -1.407
-0.013 0.014 -0.007
0.034 0.000 -0.006
-0.005 0.000 0.000

atensor 9 C
0.429 0.641 0.348
0.641 0.449 -0.002
0.348 -0.002 0.422
0.004 0.008 0.002
0.002 0.002 0.002
0.004 0.001 -0.002

atensor 10 C
0.431 -0.643 0.348
-0.643 0.447 0.003
0.348 0.003 0.419
0.004 -0.008 0.002

-0.002 0.002 -0.002
0.004 -0.002 -0.003

atensor 11 C
0.431 -0.643 -0.348
-0.643 0.447 -0.003
-0.348 -0.003 0.420
0.004 -0.008 -0.002
-0.002 0.002 0.002
-0.004 0.002 -0.003

atensor 12 C
0.429 0.641 -0.348
0.641 0.449 0.002
-0.348 0.002 0.422
0.004 0.008 -0.002
0.002 0.002 -0.002
-0.004 -0.001 -0.002

atensor 13 C
-0.188 0.489 0.459
0.489 -1.320 0.161
0.459 0.161 -1.324
0.006 0.029 0.008
0.011 -0.007 0.004
0.001 -0.001 -0.001

atensor 14 C
-0.184 -0.490 0.457
-0.490 -1.320 -0.161
0.457 -0.161 -1.324
0.006 -0.029 0.008
-0.011 -0.007 -0.004
0.001 0.001 -0.001

atensor 15 C
-0.184 -0.490 -0.458
-0.490 -1.320 0.161
-0.458 0.161 -1.324
0.006 -0.029 -0.008
-0.011 -0.007 0.004
-0.001 -0.001 -0.001

atensor 16 C
-0.188 0.489 -0.459
0.489 -1.320 -0.161
-0.459 -0.161 -1.324
0.006 0.029 -0.008
0.011 -0.007 -0.004
-0.001 0.000 -0.001

atensor 17 C
-0.032 0.233 0.063
0.233 -0.028 0.037
0.063 0.037 -0.238
0.002 0.004 0.001
0.004 0.002 0.000
0.001 0.000 -0.001

atensor 18 C
-0.031 -0.233 0.061
-0.233 -0.028 -0.036
0.062 -0.036 -0.238
0.002 -0.004 0.001
-0.004 0.002 0.000
0.001 0.000 -0.001

atensor 19 C
-0.031 -0.233 -0.062
-0.233 -0.028 0.036
-0.062 0.036 -0.238
0.002 -0.004 -0.001
-0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 20 C
-0.032 0.233 -0.063
0.233 -0.028 -0.037
-0.063 -0.037 -0.238
0.002 0.004 -0.001
0.004 0.002 0.000
-0.001 0.000 -0.001

atensor 23 C
0.170 -0.137 0.013
-0.137 0.256 -0.002
0.013 -0.002 0.049
0.000 -0.003 0.000
-0.003 0.002 0.000
0.000 0.000 -0.001

atensor 24 C
0.170 0.136 0.012
0.136 0.256 0.001
0.012 0.001 0.049
0.000 0.003 0.000
0.003 0.002 0.000
0.000 0.000 -0.001

atensor 25 C
-0.046 0.157 0.290
0.157 -0.545 -0.031
0.290 -0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 0.001
0.002 0.002 -0.001

atensor 26 C
-0.043 -0.158 0.290
-0.158 -0.544 0.031
0.290 0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 -0.001
0.002 -0.002 -0.001

atensor 27 C
-0.042 -0.158 -0.290
-0.158 -0.544 -0.031
-0.290 -0.031 -0.384
0.010 -0.007 0.000
0.003 -0.030 0.001
-0.002 0.002 -0.001

atensor 28 C
-0.046 0.157 -0.290
0.157 -0.545 0.031
-0.290 0.031 -0.385
0.010 0.007 0.000
-0.003 -0.030 -0.001
-0.002 -0.002 -0.001

atensor 29 C
0.216 0.108 0.057
0.108 0.139 0.057

0.057 0.057 0.066
0.001 0.002 0.001
0.002 0.000 0.001
0.001 0.001 -0.001

atensor 30 C
0.216 -0.108 0.057
-0.108 0.140 -0.056
0.057 -0.056 0.065
0.001 -0.002 0.001
-0.002 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.216 -0.108 -0.057
-0.108 0.140 0.056
-0.057 0.056 0.065
0.001 -0.002 -0.001
-0.002 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.216 0.108 -0.057
0.108 0.139 -0.057
-0.057 -0.057 0.066
0.001 0.002 -0.001
0.002 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.012 0.089 0.005
0.089 0.037 -0.008
0.005 -0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 34 C
0.012 -0.089 0.004
-0.089 0.037 0.008
0.004 0.008 -0.052
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 35 C
0.012 -0.089 -0.004
-0.089 0.037 -0.008
-0.004 -0.008 -0.053
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 36 C
0.012 0.089 -0.005
0.089 0.037 0.008
-0.005 0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 37 C
0.025 0.078 0.036
0.078 0.009 0.020
0.036 0.020 -0.039
0.001 0.001 0.001
0.001 0.000 0.000

0.000 0.000 0.000

atensor 38 C
0.025 -0.078 0.036
-0.078 0.009 -0.020
0.036 -0.020 -0.039
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.025 -0.078 -0.036
-0.078 0.009 0.020
-0.036 0.020 -0.039
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.025 0.078 -0.036
0.078 0.009 -0.020
-0.036 -0.020 -0.039
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.039 0.045 -0.001
0.045 0.037 0.022
-0.001 0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.039 -0.046 -0.002
-0.046 0.037 -0.021
-0.002 -0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.039 -0.046 0.002
-0.046 0.037 0.021
0.002 0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.039 0.045 0.001
0.045 0.037 -0.022
0.001 -0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.608 0.359 0.031
0.359 0.644 0.299
0.031 0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 0.006
0.000 0.002 -0.004

atensor 48 H

-0.608 -0.360 0.031
-0.360 0.645 -0.297
0.031 -0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 -0.005
0.000 -0.002 -0.004

atensor 49 H
-0.607 -0.360 -0.031
-0.360 0.645 0.297
-0.031 0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 0.005
0.000 0.002 -0.004

atensor 50 H
-0.608 0.359 -0.031
0.359 0.644 -0.299
-0.031 -0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 -0.006
0.000 -0.002 -0.004

atensor 51 H
-0.065 0.641 -0.138
0.641 0.451 -0.222
-0.138 -0.222 -0.426
-0.001 0.012 -0.003
0.012 0.009 -0.004
-0.001 -0.002 -0.004

atensor 52 H
-0.065 -0.643 -0.142
-0.643 0.451 0.227
-0.142 0.227 -0.426
-0.001 -0.012 -0.003
-0.012 0.009 0.004
-0.002 0.002 -0.004

atensor 53 H
-0.065 -0.643 0.141
-0.643 0.451 -0.227
0.141 -0.227 -0.426
-0.001 -0.012 0.003
-0.012 0.009 -0.004
0.002 -0.002 -0.004

atensor 54 H
-0.065 0.641 0.138
0.641 0.451 0.222
0.138 0.222 -0.426
-0.001 0.012 0.003
0.012 0.009 0.004
0.001 0.002 -0.004

atensor 55 H
0.237 0.433 0.408
0.433 -0.123 0.260
0.408 0.260 -0.155
0.005 0.009 0.008
0.009 -0.002 0.005
0.004 0.002 -0.001

atensor 56 H
0.238 -0.434 0.405
-0.434 -0.121 -0.259
0.405 -0.259 -0.158

0.005 -0.009 0.008
-0.009 -0.002 -0.005
0.004 -0.002 -0.001

atensor 57 H
0.238 -0.434 -0.405
-0.434 -0.121 0.259
-0.405 0.259 -0.158
0.005 -0.009 -0.008
-0.009 -0.002 0.005
-0.004 0.002 -0.001

atensor 58 H
0.237 0.433 -0.408
0.433 -0.123 -0.260
-0.408 -0.260 -0.155
0.005 0.009 -0.008
0.009 -0.002 -0.005
-0.004 -0.002 -0.001

atensor 59 H
0.026 0.235 -0.031
0.235 0.151 -0.042
-0.031 -0.042 -0.143
0.000 0.004 -0.001
0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 60 H
0.026 -0.235 -0.032
-0.235 0.151 0.044
-0.032 0.044 -0.143
0.000 -0.004 -0.001
-0.004 0.003 0.001
0.000 0.000 -0.001

atensor 61 H
0.026 -0.235 0.032
-0.235 0.151 -0.044
0.032 -0.044 -0.143
0.000 -0.004 0.001
-0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 62 H
0.026 0.235 0.031
0.235 0.151 0.042
0.031 0.042 -0.143
0.000 0.004 0.001
0.004 0.003 0.001
0.000 0.000 -0.001

atensor 63 H
0.730 0.370 0.145
0.370 -0.621 -0.001
0.145 -0.001 -0.623
0.018 0.008 0.002
0.003 -0.013 0.001
0.001 0.001 -0.005

atensor 64 H
0.733 -0.370 0.143
-0.370 -0.620 0.002
0.143 0.002 -0.622
0.018 -0.008 0.002
-0.003 -0.013 -0.001
0.001 -0.001 -0.005

atensor 65 H
0.733 -0.370 -0.143
-0.370 -0.620 -0.002
-0.143 -0.002 -0.622
0.018 -0.008 -0.002
-0.003 -0.013 0.001
-0.001 0.001 -0.005

atensor 66 H
0.730 0.370 -0.145
0.370 -0.621 0.001
-0.145 0.001 -0.623
0.018 0.008 -0.002
0.003 -0.013 -0.001
-0.001 -0.001 -0.005

atensor 67 H
0.106 0.189 0.114
0.189 0.007 0.087
0.114 0.087 -0.083
0.002 0.004 0.002
0.004 0.000 0.002
0.001 0.001 -0.001

atensor 68 H
0.106 -0.190 0.113
-0.190 0.008 -0.086
0.113 -0.086 -0.084
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.106 -0.190 -0.113
-0.190 0.008 0.086
-0.113 0.086 -0.084
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.106 0.189 -0.114
0.189 0.007 -0.087
-0.114 -0.087 -0.083
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.040 0.166 0.026
0.166 0.042 0.030
0.026 0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.040 -0.167 0.025
-0.167 0.043 -0.029
0.025 -0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.040 -0.167 -0.025

-0.167 0.042 0.029
-0.025 0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.040 0.166 -0.026
0.166 0.042 -0.030
-0.026 -0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-222.362 -17.574 -3.419
-17.574 -303.468 -44.049
-3.419 -44.049 -89.081
261.494 -4.060 -0.927
-4.060 258.056 5.856
-0.927 5.856 222.641

orbtensor 2 C
-219.822 18.349 -4.355
18.349 -305.492 43.384
-4.355 43.384 -94.639
261.477 4.036 -1.132
4.036 258.063 -5.866
-1.132 -5.866 222.651

orbtensor 3 C
-225.433 15.568 1.835
15.568 -302.935 -43.705
1.835 -43.705 -89.026
261.477 4.037 1.130
4.037 258.062 5.867
1.130 5.867 222.651

orbtensor 4 C
-221.119 -17.507 4.230
-17.507 -302.720 45.591
4.230 45.591 -88.361
261.495 -4.060 0.924
-4.060 258.056 -5.854
0.924 -5.854 222.641

orbtensor 5 C
-279.271 -8.927 1.192
-8.927 -296.354 -34.255
1.192 -34.255 -98.567
270.944 2.019 0.384
2.019 266.007 4.911
0.384 4.911 229.406

orbtensor 6 C
-281.853 9.014 1.600
9.014 -296.140 38.319
1.600 38.319 -100.112
270.956 -2.042 0.214
-2.042 266.021 -4.864
0.214 -4.864 229.412

orbtensor 7 C
-281.804 10.260 2.305
10.260 -296.000 -36.410
2.305 -36.410 -99.234
270.953 -2.041 -0.216

```

-2.041  266.019  4.867
-0.216   4.867  229.411

orbtensor 8 C
-282.637  -9.705  -1.646
-9.705 -295.389  36.978
-1.646  36.978 -98.897
270.944   2.019  -0.386
2.019  266.007  -4.910
-0.386  -4.910  229.405

orbtensor 9 C
-260.028  -16.678   3.762
-16.678 -257.763  -19.947
3.762 -19.947 -74.490
262.817   0.533   0.714
0.533  262.805   2.897
0.714   2.897  217.367

orbtensor 10 C
-258.075  16.776   2.631
16.776 -256.206  18.355
2.631  18.355 -74.760
262.813  -0.548   0.564
-0.548  262.836  -2.743
0.564  -2.743  217.353

orbtensor 11 C
-259.053  16.505  -2.329
16.505 -255.102  -18.427
-2.329 -18.427 -72.893
262.814  -0.548  -0.565
-0.548  262.834   2.745
-0.565   2.745  217.353

orbtensor 12 C
-259.644  -17.318  -2.280
-17.318 -256.759  21.007
-2.280  21.007 -72.020
262.815   0.535  -0.716
0.535  262.805  -2.893
-0.716  -2.893  217.365

orbtensor 13 C
-300.220  -10.661  19.115
-10.661 -283.140  -20.629
19.115 -20.629 -95.205
266.508   1.899  -0.234
1.899  271.118   1.929
-0.234   1.929  229.103

orbtensor 14 C
-299.361   9.261  21.554
9.261 -283.447  19.255
21.554  19.255 -96.204
266.514  -1.897  -0.276
-1.897  271.134  -1.751
-0.276  -1.751  229.095

orbtensor 15 C
-299.760   8.706  -19.523
8.706 -283.319  -18.030
-19.523  -18.030  -92.955
266.515  -1.898   0.276
-1.898  271.134   1.754
0.276   1.754  229.097

```

orbtensor 16 C
-298.786 -9.278 -19.658
-9.278 -284.538 21.670
-19.658 21.670 -91.661
266.508 1.899 0.234
1.899 271.117 -1.927
0.234 -1.927 229.102

orbtensor 17 C
-218.501 -108.469 -55.365
-108.469 -227.945 45.796
-55.365 45.796 -222.958
252.344 14.870 10.140
14.870 254.107 -8.811
10.140 -8.811 250.685

orbtensor 18 C
-218.900 107.498 -56.534
107.498 -227.150 -48.087
-56.534 -48.087 -221.677
252.384 -14.898 10.055
-14.898 254.036 8.849
10.055 8.849 250.744

orbtensor 19 C
-218.219 106.533 56.357
106.533 -228.161 46.389
56.357 46.389 -222.751
252.389 -14.894 -10.058
-14.894 254.040 -8.853
-10.058 -8.853 250.737

orbtensor 20 C
-218.946 -108.296 56.214
-108.296 -227.903 -47.905
56.214 -47.905 -224.610
252.347 14.866 -10.142
14.866 254.113 8.812
-10.142 8.812 250.685

orbtensor 23 C
-193.282 69.991 87.172
69.991 -174.808 46.914
87.172 46.914 -267.542
245.744 -15.658 -6.098
-15.658 250.614 -12.114
-6.098 -12.114 249.517

orbtensor 24 C
-193.222 -69.996 86.837
-69.996 -172.025 -47.389
86.837 -47.389 -271.332
245.733 15.657 -6.175
15.657 250.707 12.079
-6.175 12.079 249.419

orbtensor 25 C
-312.221 -16.100 23.996
-16.100 -225.653 13.001
23.996 13.001 -81.517
258.847 -4.032 -2.131
-4.032 261.430 1.193
-2.131 1.193 221.940

orbtensor 26 C
-308.989 15.571 25.399
15.571 -226.116 -12.374

25.399	-12.374	-80.989
258.850	4.042	-2.118
4.042	261.444	-0.981
-2.118	-0.981	221.933

orbtensor 27 C

-313.381	15.811	-26.469
15.811	-220.610	13.579
-26.469	13.579	-81.968
258.850	4.041	2.119
4.041	261.444	0.984
2.119	0.984	221.933

orbtensor 28 C

-308.357	-15.213	-25.179
-15.213	-225.153	-14.558
-25.179	-14.558	-81.711
258.848	-4.031	2.131
-4.031	261.430	-1.191
2.131	-1.191	221.940

orbtensor 29 C

-160.338	-73.027	-45.228
-73.027	-206.610	86.383
-45.228	86.383	-262.083
247.892	14.962	13.429
14.962	246.764	-5.422
13.429	-5.422	250.413

orbtensor 30 C

-165.514	73.669	-43.051
73.669	-205.408	-87.458
-43.051	-87.458	-265.541
247.934	-15.018	13.369
-15.018	246.724	5.428
13.369	5.428	250.400

orbtensor 31 C

-167.692	72.526	43.555
72.526	-206.088	85.026
43.555	85.026	-266.954
247.944	-15.014	-13.372
-15.014	246.724	-5.433
-13.372	-5.433	250.394

orbtensor 32 C

-164.600	-73.589	47.121
-73.589	-204.736	-87.419
47.121	-87.419	-264.097
247.893	14.959	-13.432
14.959	246.767	5.424
-13.432	5.424	250.410

orbtensor 33 C

-149.589	-78.558	-42.356
-78.558	-202.581	95.781
-42.356	95.781	-230.527
244.309	15.917	10.859
15.917	244.341	-8.472
10.859	-8.472	246.523

orbtensor 34 C

-149.043	78.293	-46.608
78.293	-204.735	-96.494
-46.608	-96.494	-229.922
244.325	-15.956	10.786
-15.956	244.272	8.486

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10.786      8.486    246.559

orbtensor 35 C
-148.248    78.835    44.117
 78.835  -199.365    96.060
 44.117    96.060  -229.443
244.333   -15.953   -10.789
-15.953   244.271    -8.492
-10.789    -8.492    246.549

orbtensor 36 C
-150.734   -76.802    43.924
-76.802  -200.921   -94.823
 43.924  -94.823  -230.340
244.310   15.915   -10.862
 15.915   244.344    8.473
-10.862    8.473    246.519

orbtensor 37 C
-180.679   -71.813   -97.804
-71.813  -160.408    40.267
-97.804   40.267  -239.556
242.783   16.010    9.546
 16.010   246.579   -9.528
 9.546   -9.528    246.312

orbtensor 38 C
-183.341    74.154   -97.089
 74.154  -158.605   -42.123
-97.089  -42.123  -238.887
242.808   -16.036    9.477
-16.036   246.515    9.553
 9.477    9.553    246.371

orbtensor 39 C
-184.573    74.452    95.093
 74.452  -159.115    43.342
 95.093   43.342  -241.405
242.816   -16.033   -9.480
-16.033   246.513   -9.558
-9.480   -9.558    246.362

orbtensor 40 C
-181.629   -74.083    97.864
-74.083  -160.492   -42.200
 97.864  -42.200  -240.278
242.782   16.008   -9.548
 16.008   246.583    9.529
-9.548    9.529    246.307

orbtensor 41 C
-196.936  -117.847   -59.621
-117.847  -210.225    46.684
-59.621   46.684  -182.806
243.819   12.806   10.666
 12.806   245.858  -10.145
 10.666  -10.145   250.687

orbtensor 42 C
-199.465   117.228   -55.692
 117.228  -212.766   -45.092
-55.692  -45.092  -184.811
243.843  -12.839   10.620
-12.839   245.775   10.140
 10.620   10.140   250.745

orbtensor 43 C

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-199.217	116.140	56.355
116.140	-210.060	45.939
56.355	45.939	-184.311
243.851	-12.835	-10.623
-12.835	245.776	-10.145
-10.623	-10.145	250.737

orbtensor 44 C

-195.774	-117.410	59.977
-117.410	-210.798	-47.139
59.977	-47.139	-182.394
243.821	12.804	-10.669
12.804	245.861	10.146
-10.669	10.146	250.684

orbtensor 47 H

-3.132	-8.254	-1.847
-8.254	-16.552	-3.152
-1.847	-3.152	-4.102
35.439	4.747	-0.170
4.747	35.614	3.098
-0.170	3.098	18.688

orbtensor 48 H

-3.225	8.325	-1.837
8.325	-16.580	3.249
-1.837	3.249	-4.359
35.436	-4.757	-0.249
-4.757	35.613	-3.062
-0.249	-3.062	18.684

orbtensor 49 H

-3.080	8.354	1.629
8.354	-16.428	-3.112
1.629	-3.112	-4.418
35.435	-4.757	0.248
-4.757	35.613	3.063
0.248	3.063	18.684

orbtensor 50 H

-3.142	-8.176	1.817
-8.176	-16.557	3.364
1.817	3.364	-4.324
35.440	4.747	0.170
4.747	35.614	-3.097
0.170	-3.097	18.688

orbtensor 51 H

-8.334	-1.466	-8.723
-1.466	-4.014	-1.782
-8.723	-1.782	-15.643
31.260	4.572	5.532
4.572	27.462	-3.734
5.532	-3.734	34.494

orbtensor 52 H

-8.488	1.578	-8.976
1.578	-3.862	2.014
-8.976	2.014	-15.525
31.262	-4.597	5.520
-4.597	27.434	3.702
5.520	3.702	34.509

orbtensor 53 H

-8.634	1.444	8.735
1.444	-3.871	-2.023
8.735	-2.023	-15.584

31.267	-4.595	-5.521
-4.595	27.434	-3.705
-5.521	-3.705	34.504

orbtensor 54 H

-8.428	-1.350	8.813
-1.350	-4.012	2.009
8.813	2.009	-15.690
31.261	4.571	-5.533
4.571	27.462	3.735
-5.533	3.735	34.492

orbtensor 55 H

-4.163	-1.396	2.952
-1.396	-9.918	9.282
2.952	9.282	-14.345
26.855	4.404	3.601
4.404	32.586	-5.339
3.601	-5.339	34.300

orbtensor 56 H

-4.020	1.385	2.885
1.385	-10.022	-9.410
2.885	-9.410	-14.435
26.872	-4.403	3.601
-4.403	32.537	5.340
3.601	5.340	34.335

orbtensor 57 H

-3.842	1.557	-2.937
1.557	-9.910	9.445
-2.937	9.445	-14.253
26.873	-4.401	-3.603
-4.401	32.539	-5.341
-3.603	-5.341	34.332

orbtensor 58 H

-4.207	-1.403	-2.964
-1.403	-10.054	-9.281
-2.964	-9.281	-14.378
26.855	4.403	-3.602
4.403	32.588	5.339
-3.602	5.339	34.299

orbtensor 59 H

-0.918	-3.151	0.573
-3.151	-9.132	8.904
0.573	8.904	-11.390
26.908	4.377	0.297
4.377	33.304	-8.823
0.297	-8.823	33.688

orbtensor 60 H

-0.979	3.142	0.597
3.142	-8.887	-8.874
0.597	-8.874	-11.734
26.901	-4.356	0.293
-4.356	33.221	8.829
0.293	8.829	33.775

orbtensor 61 H

-1.057	3.110	-0.654
3.110	-9.000	8.730
-0.654	8.730	-11.701
26.902	-4.355	-0.295
-4.355	33.223	-8.831
-0.295	-8.831	33.772

orbtensor 62 H
-0.809 -3.227 -0.592
-3.227 -9.176 -8.791
-0.592 -8.791 -11.407
26.908 4.376 -0.300
4.376 33.306 8.824
-0.300 8.824 33.686

orbtensor 63 H
-17.087 -8.540 2.464
-8.540 -3.256 1.549
2.464 1.549 -4.101
36.149 4.785 -1.310
4.785 35.224 1.178
-1.310 1.178 18.410

orbtensor 64 H
-17.014 8.543 2.394
8.543 -3.332 -1.580
2.394 -1.580 -3.846
36.157 -4.779 -1.343
-4.779 35.231 -1.090
-1.343 -1.090 18.399

orbtensor 65 H
-17.147 8.522 -2.357
8.522 -3.298 1.598
-2.357 1.598 -3.985
36.156 -4.780 1.343
-4.780 35.231 1.091
1.343 1.091 18.399

orbtensor 66 H
-17.159 -8.498 -2.368
-8.498 -3.181 -1.508
-2.368 -1.508 -3.945
36.149 4.785 1.311
4.785 35.225 -1.177
1.311 -1.177 18.410

orbtensor 67 H
-7.819 -2.326 -8.440
-2.326 -1.128 -0.024
-8.440 -0.024 -12.869
31.856 3.759 8.930
3.759 27.157 -0.500
8.930 -0.500 35.029

orbtensor 68 H
-7.795 2.296 -8.526
2.296 -1.273 0.061
-8.526 0.061 -12.834
31.890 -3.807 8.918
-3.807 27.156 0.461
8.918 0.461 34.997

orbtensor 69 H
-7.651 2.383 8.605
2.383 -1.136 -0.048
8.605 -0.048 -12.822
31.895 -3.806 -8.919
-3.806 27.155 -0.464
-8.919 -0.464 34.992

orbtensor 70 H
-7.761 -2.262 8.613

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-2.262  -1.043  -0.093
8.613   -0.093  -12.842
31.857   3.759  -8.930
3.759   27.157   0.500
-8.930   0.500   35.027

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orbtensor 71 H
-8.530  -11.264  -2.022
-11.264  -9.069   0.635
-2.022   0.635  -1.664
33.478   9.739   2.336
9.739   34.041  -1.085
2.336   -1.085  26.825

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orbtensor 72 H
-8.676  11.200  -1.929
11.200  -9.325  -0.713
-1.929  -0.713  -1.923
33.472  -9.749   2.272
-9.749  34.047   1.140
2.272   1.140  26.827

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orbtensor 73 H
-8.531  11.162   1.862
11.162  -9.259   0.704
1.862   0.704  -1.917
33.475  -9.748  -2.272
-9.748  34.044  -1.142
-2.272  -1.142  26.826

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orbtensor 74 H
-8.344  -11.343   2.094
-11.343  -8.976  -0.657
2.094   -0.657  -1.669
33.477   9.738  -2.336
9.738   34.043   1.085
-2.336   1.085  26.825

```

```

gtensor (ppt)
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000
0.000   0.000   0.000

```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4067	42.42667	210.71729	0.00000	210.71729	253.14396
2	C	-0.4097	40.74600	212.27176	0.00000	212.27176	253.01776
3	C	-0.4097	41.59867	212.27176	0.00000	212.27176	253.87043
4	C	-0.4067	43.33067	210.71729	0.00000	210.71729	254.04796
5	C	-1.1003	30.72167	570.14572	-0.00000	570.14572	600.86739
6	C	-1.0967	29.42800	568.24581	-0.00000	568.24581	597.67381
7	C	-1.0967	29.78167	568.24581	-0.00000	568.24581	598.02748
8	C	-1.1003	29.81100	570.14572	-0.00000	570.14572	599.95672
9	C	0.4347	50.23600	-225.22569	0.00000	-225.22569	-174.98969
10	C	0.4333	51.32033	-224.53482	-0.00000	-224.53482	-173.21448
11	C	0.4337	51.98433	-224.70754	0.00000	-224.70754	-172.72320
12	C	0.4347	51.52067	-225.22569	0.00000	-225.22569	-173.70503

13	C	-0.9447	29.38800	489.48590	0.00000	489.48590	518.87390
14	C	-0.9433	29.24367	488.79503	-0.00000	488.79503	518.03869
15	C	-0.9433	30.23733	488.79503	-0.00000	488.79503	519.03236
16	C	-0.9447	30.58067	489.48590	0.00000	489.48590	520.06657
17	C	-0.0983	29.24400	50.95213	0.00000	50.95213	80.19613
18	C	-0.0980	29.81233	50.77941	0.00000	50.77941	80.59175
19	C	-0.0980	29.34500	50.77941	0.00000	50.77941	80.12441
20	C	-0.0983	28.56200	50.95213	0.00000	50.95213	79.51413
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1587	36.74767	-82.21429	0.00000	-82.21429	-45.46662
24	C	0.1587	36.42667	-82.21429	0.00000	-82.21429	-45.78762
25	C	-0.3323	40.94200	172.20093	-0.00000	172.20093	213.14293
26	C	-0.3307	42.04433	171.33734	-0.00000	171.33734	213.38167
27	C	-0.3303	42.08933	171.16462	-0.00000	171.16462	213.25395
28	C	-0.3323	42.33233	172.20093	-0.00000	172.20093	214.53327
29	C	0.1403	38.67933	-72.71474	0.00000	-72.71474	-34.03540
30	C	0.1403	36.19833	-72.71474	0.00000	-72.71474	-36.51640
31	C	0.1403	34.77600	-72.71474	0.00000	-72.71474	-37.93874
32	C	0.1403	37.21233	-72.71474	0.00000	-72.71474	-35.50240
33	C	-0.0010	50.82533	0.51816	0.00000	0.51816	51.34349
34	C	-0.0007	50.48533	0.34544	0.00000	0.34544	50.83077
35	C	-0.0010	52.69900	0.51816	0.00000	0.51816	53.21716
36	C	-0.0010	51.05933	0.51816	0.00000	0.51816	51.57749
A Average		-1.0212	29.89900	529.16811	-0.00000	529.16811	559.06711
B Average		-0.3698	41.93875	191.61024	0.00000	191.61024	233.54899
M Average		0.4341	51.26533	-224.92344	0.00000	-224.92344	-173.65810

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FeL5-planar-LS-STO-PBE0-No-PSOSO

Temperature: 303

Spin: 1.5

atensor 1 C

-0.611 0.169 -0.023
0.169 -0.279 0.292
-0.023 0.292 -0.308
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 2 C

-0.614 -0.170 -0.021
-0.170 -0.282 -0.292
-0.021 -0.292 -0.311
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C

-0.614 -0.170 0.021
-0.170 -0.282 0.292
0.021 0.292 -0.311
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 C

-0.611 0.169 0.023
0.169 -0.279 -0.292
0.023 -0.292 -0.308
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C

-1.430 0.447 0.228
0.447 -0.451 0.534
0.228 0.534 -1.407
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 C
-1.425 -0.450 0.229
-0.450 -0.446 -0.533
0.229 -0.533 -1.406
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
-1.425 -0.450 -0.229
-0.450 -0.446 0.533
-0.229 0.533 -1.406
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 C
-1.430 0.447 -0.228
0.447 -0.451 -0.534
-0.228 -0.534 -1.407
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.429 0.641 0.348
0.641 0.449 -0.002
0.348 -0.002 0.422
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 C
0.431 -0.643 0.348
-0.643 0.447 0.003
0.348 0.003 0.419
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.431 -0.643 -0.348
-0.643 0.447 -0.003
-0.348 -0.003 0.420
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 C
0.429 0.641 -0.348
0.641 0.449 0.002
-0.348 0.002 0.422
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
-0.188 0.489 0.459
0.489 -1.320 0.161
0.459 0.161 -1.324

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 C
-0.184 -0.490 0.457
-0.490 -1.320 -0.161
0.457 -0.161 -1.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
-0.184 -0.490 -0.458
-0.490 -1.320 0.161
-0.458 0.161 -1.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 C
-0.188 0.489 -0.459
0.489 -1.320 -0.161
-0.459 -0.161 -1.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
-0.032 0.233 0.063
0.233 -0.028 0.037
0.063 0.037 -0.238
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.031 -0.233 0.061
-0.233 -0.028 -0.036
0.062 -0.036 -0.238
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.031 -0.233 -0.062
-0.233 -0.028 0.036
-0.062 0.036 -0.238
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.032 0.233 -0.063
0.233 -0.028 -0.037
-0.063 -0.037 -0.238
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.170 -0.137 0.013
-0.137 0.256 -0.002
0.013 -0.002 0.049
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 C
0.170 0.136 0.012
0.136 0.256 0.001
0.012 0.001 0.049
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 C
-0.046 0.157 0.290
0.157 -0.545 -0.031
0.290 -0.031 -0.385
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 C
-0.043 -0.158 0.290
-0.158 -0.544 0.031
0.290 0.031 -0.384
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 C
-0.042 -0.158 -0.290
-0.158 -0.544 -0.031
-0.290 -0.031 -0.384
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 C
-0.046 0.157 -0.290
0.157 -0.545 0.031
-0.290 0.031 -0.385
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 29 C
0.216 0.108 0.057
0.108 0.139 0.057
0.057 0.057 0.066
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.216 -0.108 0.057
-0.108 0.140 -0.056
0.057 -0.056 0.065
0.001 -0.002 0.001
-0.002 0.000 -0.001
0.001 -0.001 -0.001

atensor 31 C
0.216 -0.108 -0.057
-0.108 0.140 0.056
-0.057 0.056 0.065
0.001 -0.002 -0.001
-0.002 0.000 0.001
-0.001 0.001 -0.001

atensor 32 C
0.216 0.108 -0.057

0.108 0.139 -0.057
-0.057 -0.057 0.066
0.001 0.002 -0.001
0.002 0.000 -0.001
-0.001 -0.001 -0.001

atensor 33 C
0.012 0.089 0.005
0.089 0.037 -0.008
0.005 -0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 34 C
0.012 -0.089 0.004
-0.089 0.037 0.008
0.004 0.008 -0.052
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 35 C
0.012 -0.089 -0.004
-0.089 0.037 -0.008
-0.004 -0.008 -0.053
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 36 C
0.012 0.089 -0.005
0.089 0.037 0.008
-0.005 0.008 -0.053
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 37 C
0.025 0.078 0.036
0.078 0.009 0.020
0.036 0.020 -0.039
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.025 -0.078 0.036
-0.078 0.009 -0.020
0.036 -0.020 -0.039
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.025 -0.078 -0.036
-0.078 0.009 0.020
-0.036 0.020 -0.039
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.025 0.078 -0.036
0.078 0.009 -0.020
-0.036 -0.020 -0.039
0.001 0.001 -0.001

0.001 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.039 0.045 -0.001
0.045 0.037 0.022
-0.001 0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.039 -0.046 -0.002
-0.046 0.037 -0.021
-0.002 -0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.039 -0.046 0.002
-0.046 0.037 0.021
0.002 0.021 -0.027
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.039 0.045 0.001
0.045 0.037 -0.022
0.001 -0.022 -0.027
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.608 0.359 0.031
0.359 0.644 0.299
0.031 0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 0.006
0.000 0.002 -0.004

atensor 48 H
-0.608 -0.360 0.031
-0.360 0.645 -0.297
0.031 -0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 -0.005
0.000 -0.002 -0.004

atensor 49 H
-0.607 -0.360 -0.031
-0.360 0.645 0.297
-0.031 0.297 -0.542
-0.013 -0.003 0.000
-0.007 0.017 0.005
0.000 0.002 -0.004

atensor 50 H
-0.608 0.359 -0.031
0.359 0.644 -0.299
-0.031 -0.299 -0.542
-0.013 0.003 0.000
0.007 0.017 -0.006
0.000 -0.002 -0.004

atensor 51 H
-0.065 0.641 -0.138
0.641 0.451 -0.222
-0.138 -0.222 -0.426
-0.001 0.012 -0.003
0.012 0.009 -0.004
-0.001 -0.002 -0.004

atensor 52 H
-0.065 -0.643 -0.142
-0.643 0.451 0.227
-0.142 0.227 -0.426
-0.001 -0.012 -0.003
-0.012 0.009 0.004
-0.002 0.002 -0.004

atensor 53 H
-0.065 -0.643 0.141
-0.643 0.451 -0.227
0.141 -0.227 -0.426
-0.001 -0.012 0.003
-0.012 0.009 -0.004
0.002 -0.002 -0.004

atensor 54 H
-0.065 0.641 0.138
0.641 0.451 0.222
0.138 0.222 -0.426
-0.001 0.012 0.003
0.012 0.009 0.004
0.001 0.002 -0.004

atensor 55 H
0.237 0.433 0.408
0.433 -0.123 0.260
0.408 0.260 -0.155
0.005 0.009 0.008
0.009 -0.002 0.005
0.004 0.002 -0.001

atensor 56 H
0.238 -0.434 0.405
-0.434 -0.121 -0.259
0.405 -0.259 -0.158
0.005 -0.009 0.008
-0.009 -0.002 -0.005
0.004 -0.002 -0.001

atensor 57 H
0.238 -0.434 -0.405
-0.434 -0.121 0.259
-0.405 0.259 -0.158
0.005 -0.009 -0.008
-0.009 -0.002 0.005
-0.004 0.002 -0.001

atensor 58 H
0.237 0.433 -0.408
0.433 -0.123 -0.260
-0.408 -0.260 -0.155
0.005 0.009 -0.008
0.009 -0.002 -0.005
-0.004 -0.002 -0.001

atensor 59 H
0.026 0.235 -0.031
0.235 0.151 -0.042

-0.031 -0.042 -0.143
0.000 0.004 -0.001
0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 60 H
0.026 -0.235 -0.032
-0.235 0.151 0.044
-0.032 0.044 -0.143
0.000 -0.004 -0.001
-0.004 0.003 0.001
0.000 0.000 -0.001

atensor 61 H
0.026 -0.235 0.032
-0.235 0.151 -0.044
0.032 -0.044 -0.143
0.000 -0.004 0.001
-0.004 0.003 -0.001
0.000 0.000 -0.001

atensor 62 H
0.026 0.235 0.031
0.235 0.151 0.042
0.031 0.042 -0.143
0.000 0.004 0.001
0.004 0.003 0.001
0.000 0.000 -0.001

atensor 63 H
0.730 0.370 0.145
0.370 -0.621 -0.001
0.145 -0.001 -0.623
0.018 0.008 0.002
0.003 -0.013 0.001
0.001 0.001 -0.005

atensor 64 H
0.733 -0.370 0.143
-0.370 -0.620 0.002
0.143 0.002 -0.622
0.018 -0.008 0.002
-0.003 -0.013 -0.001
0.001 -0.001 -0.005

atensor 65 H
0.733 -0.370 -0.143
-0.370 -0.620 -0.002
-0.143 -0.002 -0.622
0.018 -0.008 -0.002
-0.003 -0.013 0.001
-0.001 0.001 -0.005

atensor 66 H
0.730 0.370 -0.145
0.370 -0.621 0.001
-0.145 0.001 -0.623
0.018 0.008 -0.002
0.003 -0.013 -0.001
-0.001 -0.001 -0.005

atensor 67 H
0.106 0.189 0.114
0.189 0.007 0.087
0.114 0.087 -0.083
0.002 0.004 0.002
0.004 0.000 0.002

0.001 0.001 -0.001

atensor 68 H
0.106 -0.190 0.113
-0.190 0.008 -0.086
0.113 -0.086 -0.084
0.002 -0.004 0.002
-0.004 0.000 -0.002
0.001 -0.001 -0.001

atensor 69 H
0.106 -0.190 -0.113
-0.190 0.008 0.086
-0.113 0.086 -0.084
0.002 -0.004 -0.002
-0.004 0.000 0.002
-0.001 0.001 -0.001

atensor 70 H
0.106 0.189 -0.114
0.189 0.007 -0.087
-0.114 -0.087 -0.083
0.002 0.004 -0.002
0.004 0.000 -0.002
-0.001 -0.001 -0.001

atensor 71 H
0.040 0.166 0.026
0.166 0.042 0.030
0.026 0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

atensor 72 H
0.040 -0.167 0.025
-0.167 0.043 -0.029
0.025 -0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 73 H
0.040 -0.167 -0.025
-0.167 0.042 0.029
-0.025 0.029 -0.124
0.001 -0.003 0.000
-0.003 0.001 0.000
0.000 0.000 -0.001

atensor 74 H
0.040 0.166 -0.026
0.166 0.042 -0.030
-0.026 -0.030 -0.124
0.001 0.003 0.000
0.003 0.001 0.000
0.000 0.000 -0.001

orbtensor 1 C
-222.362 -17.574 -3.419
-17.574 -303.468 -44.049
-3.419 -44.049 -89.081
261.494 -4.060 -0.927
-4.060 258.056 5.856
-0.927 5.856 222.641

orbtensor 2 C

```
-219.822  18.349  -4.355
18.349 -305.492  43.384
-4.355  43.384 -94.639
261.477  4.036  -1.132
4.036  258.063  -5.866
-1.132  -5.866  222.651
```

```
orbtensor 3 C
-225.433  15.568  1.835
15.568 -302.935  -43.705
1.835 -43.705 -89.026
261.477  4.037  1.130
4.037  258.062  5.867
1.130  5.867  222.651
```

```
orbtensor 4 C
-221.119  -17.507  4.230
-17.507 -302.720  45.591
4.230  45.591 -88.361
261.495  -4.060  0.924
-4.060  258.056  -5.854
0.924  -5.854  222.641
```

```
orbtensor 5 C
-279.271  -8.927  1.192
-8.927 -296.354  -34.255
1.192 -34.255 -98.567
270.944  2.019  0.384
2.019  266.007  4.911
0.384  4.911  229.406
```

```
orbtensor 6 C
-281.853  9.014  1.600
9.014 -296.140  38.319
1.600  38.319 -100.112
270.956  -2.042  0.214
-2.042  266.021  -4.864
0.214  -4.864  229.412
```

```
orbtensor 7 C
-281.804  10.260  2.305
10.260 -296.000  -36.410
2.305 -36.410 -99.234
270.953  -2.041  -0.216
-2.041  266.019  4.867
-0.216  4.867  229.411
```

```
orbtensor 8 C
-282.637  -9.705  -1.646
-9.705 -295.389  36.978
-1.646  36.978 -98.897
270.944  2.019  -0.386
2.019  266.007  -4.910
-0.386  -4.910  229.405
```

```
orbtensor 9 C
-260.028  -16.678  3.762
-16.678 -257.763  -19.947
3.762 -19.947 -74.490
262.817  0.533  0.714
0.533  262.805  2.897
0.714  2.897  217.367
```

```
orbtensor 10 C
-258.075  16.776  2.631
16.776 -256.206  18.355
2.631  18.355  -74.760
```

262.813 -0.548 0.564
-0.548 262.836 -2.743
0.564 -2.743 217.353

orbtensor 11 C
-259.053 16.505 -2.329
16.505 -255.102 -18.427
-2.329 -18.427 -72.893
262.814 -0.548 -0.565
-0.548 262.834 2.745
-0.565 2.745 217.353

orbtensor 12 C
-259.644 -17.318 -2.280
-17.318 -256.759 21.007
-2.280 21.007 -72.020
262.815 0.535 -0.716
0.535 262.805 -2.893
-0.716 -2.893 217.365

orbtensor 13 C
-300.220 -10.661 19.115
-10.661 -283.140 -20.629
19.115 -20.629 -95.205
266.508 1.899 -0.234
1.899 271.118 1.929
-0.234 1.929 229.103

orbtensor 14 C
-299.361 9.261 21.554
9.261 -283.447 19.255
21.554 19.255 -96.204
266.514 -1.897 -0.276
-1.897 271.134 -1.751
-0.276 -1.751 229.095

orbtensor 15 C
-299.760 8.706 -19.523
8.706 -283.319 -18.030
-19.523 -18.030 -92.955
266.515 -1.898 0.276
-1.898 271.134 1.754
0.276 1.754 229.097

orbtensor 16 C
-298.786 -9.278 -19.658
-9.278 -284.538 21.670
-19.658 21.670 -91.661
266.508 1.899 0.234
1.899 271.117 -1.927
0.234 -1.927 229.102

orbtensor 17 C
-218.501 -108.469 -55.365
-108.469 -227.945 45.796
-55.365 45.796 -222.958
252.344 14.870 10.140
14.870 254.107 -8.811
10.140 -8.811 250.685

orbtensor 18 C
-218.900 107.498 -56.534
107.498 -227.150 -48.087
-56.534 -48.087 -221.677
252.384 -14.898 10.055
-14.898 254.036 8.849
10.055 8.849 250.744

orbtensor 19 C
-218.219 106.533 56.357
106.533 -228.161 46.389
56.357 46.389 -222.751
252.389 -14.894 -10.058
-14.894 254.040 -8.853
-10.058 -8.853 250.737

orbtensor 20 C
-218.946 -108.296 56.214
-108.296 -227.903 -47.905
56.214 -47.905 -224.610
252.347 14.866 -10.142
14.866 254.113 8.812
-10.142 8.812 250.685

orbtensor 23 C
-193.282 69.991 87.172
69.991 -174.808 46.914
87.172 46.914 -267.542
245.744 -15.658 -6.098
-15.658 250.614 -12.114
-6.098 -12.114 249.517

orbtensor 24 C
-193.222 -69.996 86.837
-69.996 -172.025 -47.389
86.837 -47.389 -271.332
245.733 15.657 -6.175
15.657 250.707 12.079
-6.175 12.079 249.419

orbtensor 25 C
-312.221 -16.100 23.996
-16.100 -225.653 13.001
23.996 13.001 -81.517
258.847 -4.032 -2.131
-4.032 261.430 1.193
-2.131 1.193 221.940

orbtensor 26 C
-308.989 15.571 25.399
15.571 -226.116 -12.374
25.399 -12.374 -80.989
258.850 4.042 -2.118
4.042 261.444 -0.981
-2.118 -0.981 221.933

orbtensor 27 C
-313.381 15.811 -26.469
15.811 -220.610 13.579
-26.469 13.579 -81.968
258.850 4.041 2.119
4.041 261.444 0.984
2.119 0.984 221.933

orbtensor 28 C
-308.357 -15.213 -25.179
-15.213 -225.153 -14.558
-25.179 -14.558 -81.711
258.848 -4.031 2.131
-4.031 261.430 -1.191
2.131 -1.191 221.940

orbtensor 29 C
-160.338 -73.027 -45.228

-73.027	-206.610	86.383
-45.228	86.383	-262.083
247.892	14.962	13.429
14.962	246.764	-5.422
13.429	-5.422	250.413

orbtensor 30 C

-165.514	73.669	-43.051
73.669	-205.408	-87.458
-43.051	-87.458	-265.541
247.934	-15.018	13.369
-15.018	246.724	5.428
13.369	5.428	250.400

orbtensor 31 C

-167.692	72.526	43.555
72.526	-206.088	85.026
43.555	85.026	-266.954
247.944	-15.014	-13.372
-15.014	246.724	-5.433
-13.372	-5.433	250.394

orbtensor 32 C

-164.600	-73.589	47.121
-73.589	-204.736	-87.419
47.121	-87.419	-264.097
247.893	14.959	-13.432
14.959	246.767	5.424
-13.432	5.424	250.410

orbtensor 33 C

-149.589	-78.558	-42.356
-78.558	-202.581	95.781
-42.356	95.781	-230.527
244.309	15.917	10.859
15.917	244.341	-8.472
10.859	-8.472	246.523

orbtensor 34 C

-149.043	78.293	-46.608
78.293	-204.735	-96.494
-46.608	-96.494	-229.922
244.325	-15.956	10.786
-15.956	244.272	8.486
10.786	8.486	246.559

orbtensor 35 C

-148.248	78.835	44.117
78.835	-199.365	96.060
44.117	96.060	-229.443
244.333	-15.953	-10.789
-15.953	244.271	-8.492
-10.789	-8.492	246.549

orbtensor 36 C

-150.734	-76.802	43.924
-76.802	-200.921	-94.823
43.924	-94.823	-230.340
244.310	15.915	-10.862
15.915	244.344	8.473
-10.862	8.473	246.519

orbtensor 37 C

-180.679	-71.813	-97.804
-71.813	-160.408	40.267
-97.804	40.267	-239.556
242.783	16.010	9.546

16.010 246.579 -9.528
9.546 -9.528 246.312

orbtensor 38 C
-183.341 74.154 -97.089
74.154 -158.605 -42.123
-97.089 -42.123 -238.887
242.808 -16.036 9.477
-16.036 246.515 9.553
9.477 9.553 246.371

orbtensor 39 C
-184.573 74.452 95.093
74.452 -159.115 43.342
95.093 43.342 -241.405
242.816 -16.033 -9.480
-16.033 246.513 -9.558
-9.480 -9.558 246.362

orbtensor 40 C
-181.629 -74.083 97.864
-74.083 -160.492 -42.200
97.864 -42.200 -240.278
242.782 16.008 -9.548
16.008 246.583 9.529
-9.548 9.529 246.307

orbtensor 41 C
-196.936 -117.847 -59.621
-117.847 -210.225 46.684
-59.621 46.684 -182.806
243.819 12.806 10.666
12.806 245.858 -10.145
10.666 -10.145 250.687

orbtensor 42 C
-199.465 117.228 -55.692
117.228 -212.766 -45.092
-55.692 -45.092 -184.811
243.843 -12.839 10.620
-12.839 245.775 10.140
10.620 10.140 250.745

orbtensor 43 C
-199.217 116.140 56.355
116.140 -210.060 45.939
56.355 45.939 -184.311
243.851 -12.835 -10.623
-12.835 245.776 -10.145
-10.623 -10.145 250.737

orbtensor 44 C
-195.774 -117.410 59.977
-117.410 -210.798 -47.139
59.977 -47.139 -182.394
243.821 12.804 -10.669
12.804 245.861 10.146
-10.669 10.146 250.684

orbtensor 47 H
-3.132 -8.254 -1.847
-8.254 -16.552 -3.152
-1.847 -3.152 -4.102
35.439 4.747 -0.170
4.747 35.614 3.098
-0.170 3.098 18.688

orbtensor 48 H
-3.225 8.325 -1.837
8.325 -16.580 3.249
-1.837 3.249 -4.359
35.436 -4.757 -0.249
-4.757 35.613 -3.062
-0.249 -3.062 18.684

orbtensor 49 H
-3.080 8.354 1.629
8.354 -16.428 -3.112
1.629 -3.112 -4.418
35.435 -4.757 0.248
-4.757 35.613 3.063
0.248 3.063 18.684

orbtensor 50 H
-3.142 -8.176 1.817
-8.176 -16.557 3.364
1.817 3.364 -4.324
35.440 4.747 0.170
4.747 35.614 -3.097
0.170 -3.097 18.688

orbtensor 51 H
-8.334 -1.466 -8.723
-1.466 -4.014 -1.782
-8.723 -1.782 -15.643
31.260 4.572 5.532
4.572 27.462 -3.734
5.532 -3.734 34.494

orbtensor 52 H
-8.488 1.578 -8.976
1.578 -3.862 2.014
-8.976 2.014 -15.525
31.262 -4.597 5.520
-4.597 27.434 3.702
5.520 3.702 34.509

orbtensor 53 H
-8.634 1.444 8.735
1.444 -3.871 -2.023
8.735 -2.023 -15.584
31.267 -4.595 -5.521
-4.595 27.434 -3.705
-5.521 -3.705 34.504

orbtensor 54 H
-8.428 -1.350 8.813
-1.350 -4.012 2.009
8.813 2.009 -15.690
31.261 4.571 -5.533
4.571 27.462 3.735
-5.533 3.735 34.492

orbtensor 55 H
-4.163 -1.396 2.952
-1.396 -9.918 9.282
2.952 9.282 -14.345
26.855 4.404 3.601
4.404 32.586 -5.339
3.601 -5.339 34.300

orbtensor 56 H
-4.020 1.385 2.885
1.385 -10.022 -9.410

2.885	-9.410	-14.435
26.872	-4.403	3.601
-4.403	32.537	5.340
3.601	5.340	34.335

orbtensor 57 H

-3.842	1.557	-2.937
1.557	-9.910	9.445
-2.937	9.445	-14.253
26.873	-4.401	-3.603
-4.401	32.539	-5.341
-3.603	-5.341	34.332

orbtensor 58 H

-4.207	-1.403	-2.964
-1.403	-10.054	-9.281
-2.964	-9.281	-14.378
26.855	4.403	-3.602
4.403	32.588	5.339
-3.602	5.339	34.299

orbtensor 59 H

-0.918	-3.151	0.573
-3.151	-9.132	8.904
0.573	8.904	-11.390
26.908	4.377	0.297
4.377	33.304	-8.823
0.297	-8.823	33.688

orbtensor 60 H

-0.979	3.142	0.597
3.142	-8.887	-8.874
0.597	-8.874	-11.734
26.901	-4.356	0.293
-4.356	33.221	8.829
0.293	8.829	33.775

orbtensor 61 H

-1.057	3.110	-0.654
3.110	-9.000	8.730
-0.654	8.730	-11.701
26.902	-4.355	-0.295
-4.355	33.223	-8.831
-0.295	-8.831	33.772

orbtensor 62 H

-0.809	-3.227	-0.592
-3.227	-9.176	-8.791
-0.592	-8.791	-11.407
26.908	4.376	-0.300
4.376	33.306	8.824
-0.300	8.824	33.686

orbtensor 63 H

-17.087	-8.540	2.464
-8.540	-3.256	1.549
2.464	1.549	-4.101
36.149	4.785	-1.310
4.785	35.224	1.178
-1.310	1.178	18.410

orbtensor 64 H

-17.014	8.543	2.394
8.543	-3.332	-1.580
2.394	-1.580	-3.846
36.157	-4.779	-1.343
-4.779	35.231	-1.090

-1.343 -1.090 18.399

orbtensor 65 H

-17.147 8.522 -2.357
8.522 -3.298 1.598
-2.357 1.598 -3.985
36.156 -4.780 1.343
-4.780 35.231 1.091
1.343 1.091 18.399

orbtensor 66 H

-17.159 -8.498 -2.368
-8.498 -3.181 -1.508
-2.368 -1.508 -3.945
36.149 4.785 1.311
4.785 35.225 -1.177
1.311 -1.177 18.410

orbtensor 67 H

-7.819 -2.326 -8.440
-2.326 -1.128 -0.024
-8.440 -0.024 -12.869
31.856 3.759 8.930
3.759 27.157 -0.500
8.930 -0.500 35.029

orbtensor 68 H

-7.795 2.296 -8.526
2.296 -1.273 0.061
-8.526 0.061 -12.834
31.890 -3.807 8.918
-3.807 27.156 0.461
8.918 0.461 34.997

orbtensor 69 H

-7.651 2.383 8.605
2.383 -1.136 -0.048
8.605 -0.048 -12.822
31.895 -3.806 -8.919
-3.806 27.155 -0.464
-8.919 -0.464 34.992

orbtensor 70 H

-7.761 -2.262 8.613
-2.262 -1.043 -0.093
8.613 -0.093 -12.842
31.857 3.759 -8.930
3.759 27.157 0.500
-8.930 0.500 35.027

orbtensor 71 H

-8.530 -11.264 -2.022
-11.264 -9.069 0.635
-2.022 0.635 -1.664
33.478 9.739 2.336
9.739 34.041 -1.085
2.336 -1.085 26.825

orbtensor 72 H

-8.676 11.200 -1.929
11.200 -9.325 -0.713
-1.929 -0.713 -1.923
33.472 -9.749 2.272
-9.749 34.047 1.140
2.272 1.140 26.827

orbtensor 73 H

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-8.531  11.162  1.862
11.162  -9.259  0.704
1.862   0.704  -1.917
33.475  -9.748  -2.272
-9.748  34.044  -1.142
-2.272  -1.142  26.826

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orbtensor 74 H
-8.344  -11.343  2.094
-11.343  -8.976  -0.657
2.094   -0.657  -1.669
33.477   9.738  -2.336
9.738   34.043  1.085
-2.336   1.085  26.825

```

```

gtensor (ppt)
0.000  0.000  0.000
0.000  0.000  0.000
0.000  0.000  0.000
0.000  0.000  0.000
0.000  0.000  0.000
0.000  0.000  0.000

```

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.3993	42.42667	206.91747	0.00000	206.91747	249.34414
2	C	-0.4023	40.74600	208.47194	0.00000	208.47194	249.21794
3	C	-0.4023	41.59867	208.47194	0.00000	208.47194	250.07061
4	C	-0.3993	43.33067	206.91747	0.00000	206.91747	250.24814
5	C	-1.0960	30.72167	567.90037	-0.00000	567.90037	598.62204
6	C	-1.0923	29.42800	566.00046	-0.00000	566.00046	595.42846
7	C	-1.0923	29.78167	566.00046	-0.00000	566.00046	595.78213
8	C	-1.0960	29.81100	567.90037	-0.00000	567.90037	597.71137
9	C	0.4333	50.23600	-224.53482	0.00000	-224.53482	-174.29882
10	C	0.4323	51.32033	-224.01666	-0.00000	-224.01666	-172.69633
11	C	0.4327	51.98433	-224.18938	0.00000	-224.18938	-172.20505
12	C	0.4333	51.52067	-224.53482	0.00000	-224.53482	-173.01415
13	C	-0.9440	29.38800	489.14047	0.00000	489.14047	518.52847
14	C	-0.9427	29.24367	488.44959	-0.00000	488.44959	517.69326
15	C	-0.9427	30.23733	488.44959	-0.00000	488.44959	518.68692
16	C	-0.9440	30.58067	489.14047	0.00000	489.14047	519.72113
17	C	-0.0993	29.24400	51.47029	0.00000	51.47029	80.71429
18	C	-0.0990	29.81233	51.29757	0.00000	51.29757	81.10990
19	C	-0.0990	29.34500	51.29757	0.00000	51.29757	80.64257
20	C	-0.0993	28.56200	51.47029	0.00000	51.47029	80.03229
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1583	36.74767	-82.04157	0.00000	-82.04157	-45.29390
24	C	0.1583	36.42667	-82.04157	0.00000	-82.04157	-45.61490
25	C	-0.3253	40.94200	168.57383	-0.00000	168.57383	209.51583
26	C	-0.3237	42.04433	167.71024	-0.00000	167.71024	209.75457
27	C	-0.3233	42.08933	167.53752	-0.00000	167.53752	209.62685
28	C	-0.3253	42.33233	168.57383	-0.00000	168.57383	210.90617
29	C	0.1403	38.67933	-72.71474	0.00000	-72.71474	-34.03540
30	C	0.1403	36.19833	-72.71474	0.00000	-72.71474	-36.51640
31	C	0.1403	34.77600	-72.71474	0.00000	-72.71474	-37.93874
32	C	0.1403	37.21233	-72.71474	0.00000	-72.71474	-35.50240
33	C	-0.0010	50.82533	0.51816	0.00000	0.51816	51.34349
34	C	-0.0007	50.48533	0.34544	0.00000	0.34544	50.83077
35	C	-0.0010	52.69900	0.51816	0.00000	0.51816	53.21716

36	C	-0.0010	51.05933	0.51816	0.00000	0.51816	51.57749
A Average		-1.0188	29.89900	527.87272	-0.00000	527.87272	557.77172
B Average		-0.3626	41.93875	187.89678	0.00000	187.89678	229.83553
M Average		0.4329	51.26533	-224.31892	0.00000	-224.31892	-173.05359

=====
 FeL5-planar-LS-STO-PBE0-No-ZORA
 Temperature: 303
 Spin: 1.5

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	-0.4030	42.42667	208.81738	-0.00000	208.81738	251.24405
2	C	-0.4070	40.74600	210.89001	-0.00000	210.89001	251.63601
3	C	-0.4067	41.59867	210.71729	-0.00000	210.71729	252.31596
4	C	-0.4030	43.33067	208.81738	-0.00000	208.81738	252.14805
5	C	-1.0927	30.72167	566.17318	0.00000	566.17318	596.89485
6	C	-1.0890	29.42800	564.27327	0.00000	564.27327	593.70127
7	C	-1.0890	29.78167	564.27327	0.00000	564.27327	594.05494
8	C	-1.0927	29.81100	566.17318	0.00000	566.17318	595.98418
9	C	0.4187	50.23600	-216.93518	0.00000	-216.93518	-166.69918
10	C	0.4177	51.32033	-216.41702	0.00000	-216.41702	-165.09669
11	C	0.4177	51.98433	-216.41702	0.00000	-216.41702	-164.43269
12	C	0.4187	51.52067	-216.93518	0.00000	-216.93518	-165.41451
13	C	-0.9363	29.38800	485.16793	0.00000	485.16793	514.55593
14	C	-0.9353	29.24367	484.64977	0.00000	484.64977	513.89344
15	C	-0.9353	30.23733	484.64977	0.00000	484.64977	514.88710
16	C	-0.9363	30.58067	485.16793	0.00000	485.16793	515.74859
17	C	-0.0847	29.24400	43.87065	0.00000	43.87065	73.11465
18	C	-0.0843	29.81233	43.69793	0.00000	43.69793	73.51026
19	C	-0.0843	29.34500	43.69793	0.00000	43.69793	73.04293
20	C	-0.0847	28.56200	43.87065	0.00000	43.87065	72.43265
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.1453	36.74767	-75.30552	0.00000	-75.30552	-38.55786
24	C	0.1450	36.42667	-75.13280	0.00000	-75.13280	-38.70614
25	C	-0.3420	40.94200	177.20979	0.00000	177.20979	218.15179
26	C	-0.3397	42.04433	176.00075	-0.00000	176.00075	218.04509
27	C	-0.3397	42.08933	176.00075	-0.00000	176.00075	218.09009
28	C	-0.3420	42.33233	177.20979	0.00000	177.20979	219.54212
29	C	0.1250	38.67933	-64.76966	0.00000	-64.76966	-26.09033
30	C	0.1247	36.19833	-64.59694	-0.00000	-64.59694	-28.39861
31	C	0.1247	34.77600	-64.59694	-0.00000	-64.59694	-29.82094
32	C	0.1250	37.21233	-64.76966	0.00000	-64.76966	-27.55733
33	C	-0.0017	50.82533	0.86360	0.00000	0.86360	51.68893
34	C	-0.0013	50.48533	0.69088	0.00000	0.69088	51.17621
35	C	-0.0013	52.69900	0.69088	0.00000	0.69088	53.38988
36	C	-0.0017	51.05933	0.86360	0.00000	0.86360	51.92293
A Average		-1.0133	29.89900	525.06604	0.00000	525.06604	554.96504
B Average		-0.3729	41.93875	193.20789	-0.00000	193.20789	235.14664
M Average		0.4182	51.26533	-216.67610	0.00000	-216.67610	-165.41077

=====
 FeL5-planar-HS-STO-PBE0-Full-Finite
 Temperature: 303
 Spin: 2.5

atensor 1 C
 0.754 0.070 0.015
 0.070 1.541 0.154
 0.015 0.154 0.831
 -0.009 -0.001 0.000

0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C
0.754 -0.071 0.016
-0.071 1.540 -0.154
0.016 -0.154 0.830
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C
0.754 -0.071 -0.016
-0.071 1.540 0.154
-0.016 0.154 0.830
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.754 0.070 -0.015
0.070 1.541 -0.154
-0.015 -0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.746 0.807 0.148
0.807 1.849 0.397
0.148 0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 0.001
0.000 0.001 0.002

atensor 6 C
0.742 -0.808 0.144
-0.808 1.846 -0.394
0.144 -0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 7 C
0.742 -0.808 -0.144
-0.808 1.846 0.394
-0.144 0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 0.001
0.000 0.001 0.002

atensor 8 C
0.746 0.807 -0.148
0.807 1.849 -0.397
-0.148 -0.397 -0.042
-0.003 0.005 0.000
0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 9 C
0.210 0.590 0.152
0.590 0.210 0.119
0.152 0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 0.001
0.002 0.000 0.000

atensor 10 C
0.211 -0.591 0.153
-0.591 0.210 -0.119
0.153 -0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 -0.001
0.002 0.000 0.000

atensor 11 C
0.211 -0.591 -0.153
-0.591 0.210 0.119
-0.153 0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 0.001
-0.002 0.000 0.000

atensor 12 C
0.210 0.590 -0.152
0.590 0.210 -0.119
-0.152 -0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 -0.001
-0.002 0.000 0.000

atensor 13 C
1.880 0.825 0.244
0.825 0.723 0.098
0.244 0.098 -0.088
0.003 0.007 0.001
0.005 -0.002 0.000
0.001 -0.001 0.001

atensor 14 C
1.880 -0.825 0.240
-0.825 0.719 -0.094
0.240 -0.094 -0.091
0.003 -0.007 0.001
-0.005 -0.002 0.000
0.001 0.001 0.001

atensor 15 C
1.880 -0.825 -0.240
-0.825 0.719 0.094
-0.240 0.094 -0.091
0.003 -0.007 -0.001
-0.005 -0.002 0.000
-0.001 -0.001 0.001

atensor 16 C
1.880 0.825 -0.244
0.825 0.723 -0.098
-0.244 -0.098 -0.087
0.003 0.007 -0.001
0.004 -0.002 0.000
-0.001 0.001 0.001

atensor 17 C
-0.106 0.239 0.060
0.239 -0.103 0.029
0.060 0.029 -0.323
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.106 -0.239 0.059
-0.239 -0.103 -0.028

0.059 -0.028 -0.324
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.106 -0.239 -0.059
-0.239 -0.103 0.028
-0.059 0.028 -0.324
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.106 0.239 -0.060
0.239 -0.103 -0.029
-0.060 -0.029 -0.323
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.216 -0.135 0.019
-0.135 0.318 -0.011
0.019 -0.011 0.089
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.215 0.135 0.018
0.135 0.317 0.009
0.018 0.009 0.088
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.562 0.078 0.038
0.078 0.727 0.023
0.038 0.023 0.763
0.002 -0.001 0.001
0.000 -0.009 0.000
0.001 0.001 -0.001

atensor 26 C
1.561 -0.077 0.038
-0.077 0.725 -0.023
0.038 -0.023 0.761
0.002 0.001 0.001
0.000 -0.009 0.000
0.001 -0.001 -0.001

atensor 27 C
1.561 -0.077 -0.038
-0.077 0.725 0.023
-0.038 0.023 0.761
0.002 0.001 -0.001
0.000 -0.009 0.000
-0.001 0.001 -0.001

atensor 28 C
1.562 0.078 -0.038
0.078 0.727 -0.023
-0.038 -0.023 0.763
0.002 -0.001 -0.001
0.000 -0.009 0.000

-0.001 -0.001 -0.001

atensor 29 C
0.290 0.111 0.061
0.111 0.197 0.059
0.061 0.059 0.114
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.290 -0.111 0.060
-0.111 0.197 -0.058
0.060 -0.058 0.114
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.290 -0.111 -0.060
-0.111 0.197 0.058
-0.060 0.058 0.114
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.290 0.111 -0.061
0.111 0.197 -0.059
-0.061 -0.059 0.114
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.020 0.092 0.003
0.092 0.046 -0.011
0.003 -0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.021 -0.092 0.002
-0.092 0.046 0.011
0.002 0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.021 -0.092 -0.002
-0.092 0.046 -0.011
-0.002 -0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.020 0.092 -0.003
0.092 0.046 0.011
-0.003 0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C

```
-222.856  -15.441  -1.797
-15.441  -302.054  -41.543
-1.797   -41.543  -87.648
261.510   -4.054   -0.922
-4.054   258.053   5.920
-0.922    5.920   222.696
```

```
orbtensor 2 C
-223.014   16.761    2.778
16.761  -299.984   41.884
2.778   41.884  -88.196
261.493    4.030   -1.127
4.030   258.060  -5.929
-1.127   -5.929   222.705
```

```
orbtensor 3 C
-223.132   16.202   -1.526
16.202  -300.516  -39.721
-1.526  -39.721  -89.594
261.493    4.030    1.125
4.030   258.060    5.931
1.125    5.931   222.706
```

```
orbtensor 4 C
-222.803  -16.997    0.252
-16.997  -301.519   44.429
0.252   44.429  -89.167
261.510   -4.053    0.920
-4.053   258.053  -5.918
0.920   -5.918   222.695
```

```
orbtensor 5 C
-283.518   -6.839   -2.496
-6.839  -297.188  -32.053
-2.496  -32.053  -109.849
270.694    2.204    0.455
2.204   265.836    4.951
0.455    4.951   228.872
```

```
orbtensor 6 C
-283.169    6.751    0.022
6.751  -293.464   34.072
0.022   34.072  -108.487
270.708   -2.227    0.285
-2.227   265.850  -4.902
0.285   -4.902   228.878
```

```
orbtensor 7 C
-281.417    5.524    2.548
5.524  -296.065  -33.489
2.548  -33.489  -111.853
270.706   -2.226   -0.286
-2.226   265.848    4.905
-0.286    4.905   228.877
```

```
orbtensor 8 C
-281.753   -6.301    0.116
-6.301  -296.147   33.055
0.116   33.055  -113.589
270.695    2.204   -0.457
2.204   265.836  -4.950
-0.457   -4.950   228.871
```

```
orbtensor 9 C
-256.114  -12.899    4.949
-12.899  -256.778  -21.424
4.949   -21.424  -75.935
```

262.817	0.522	0.776
0.522	262.852	2.900
0.776	2.900	217.332

orbtensor 10 C

-257.018	10.847	3.512
10.847	-258.260	20.675
3.512	20.675	-76.929
262.813	-0.536	0.627
-0.536	262.882	-2.748
0.627	-2.748	217.318

orbtensor 11 C

-258.134	12.197	-6.781
12.197	-257.286	-21.930
-6.781	-21.930	-76.167
262.814	-0.536	-0.628
-0.536	262.880	2.750
-0.628	2.750	217.318

orbtensor 12 C

-256.347	-11.281	-1.707
-11.281	-256.573	21.351
-1.707	21.351	-73.763
262.815	0.523	-0.778
0.523	262.852	-2.897
-0.778	-2.897	217.330

orbtensor 13 C

-298.065	-6.412	12.362
-6.412	-286.327	-3.750
12.362	-3.750	-107.790
266.304	2.067	-0.214
2.067	270.874	1.957
-0.214	1.957	228.568

orbtensor 14 C

-298.237	7.973	13.123
7.973	-284.550	3.905
13.123	3.905	-108.512
266.311	-2.065	-0.257
-2.065	270.892	-1.778
-0.257	-1.778	228.561

orbtensor 15 C

-299.216	7.653	-14.399
7.653	-283.915	-8.652
-14.399	-8.652	-104.072
266.312	-2.066	0.257
-2.066	270.892	1.781
0.257	1.781	228.563

orbtensor 16 C

-298.254	-5.534	-14.430
-5.534	-284.064	5.084
-14.430	5.084	-104.682
266.304	2.067	0.214
2.067	270.874	-1.954
0.214	-1.954	228.568

orbtensor 17 C

-217.551	-106.228	-56.647
-106.228	-227.046	47.957
-56.647	47.957	-217.887
252.329	14.873	10.149
14.873	254.103	-8.807
10.149	-8.807	250.659

orbtensor 18 C
-217.075 106.962 -55.380
106.962 -226.613 -48.087
-55.380 -48.087 -220.922
252.369 -14.901 10.063
-14.901 254.033 8.845
10.063 8.845 250.718

orbtensor 19 C
-220.287 107.565 57.620
107.565 -228.946 46.452
57.620 46.452 -220.680
252.374 -14.897 -10.067
-14.897 254.036 -8.849
-10.067 -8.849 250.712

orbtensor 20 C
-220.317 -108.397 55.496
-108.397 -228.227 -47.598
55.496 -47.598 -221.872
252.332 14.869 -10.151
14.869 254.109 8.809
-10.151 8.809 250.660

orbtensor 23 C
-189.408 69.892 85.922
69.892 -172.383 44.923
85.922 44.923 -269.970
245.741 -15.658 -6.123
-15.658 250.597 -12.110
-6.123 -12.110 249.496

orbtensor 24 C
-190.533 -70.911 85.463
-70.911 -171.824 -45.361
85.463 -45.361 -272.059
245.730 15.657 -6.199
15.657 250.691 12.075
-6.199 12.075 249.398

orbtensor 25 C
-307.696 -16.097 21.744
-16.097 -225.894 7.542
21.744 7.542 -85.351
258.883 -4.015 -2.040
-4.015 261.443 1.187
-2.040 1.187 221.963

orbtensor 26 C
-309.811 13.676 22.442
13.676 -221.257 -4.335
22.442 -4.335 -87.456
258.886 4.025 -2.027
4.025 261.456 -0.975
-2.027 -0.975 221.956

orbtensor 27 C
-308.240 14.531 -23.321
14.531 -219.568 9.035
-23.321 9.035 -87.052
258.887 4.024 2.029
4.024 261.456 0.978
2.029 0.978 221.955

orbtensor 28 C
-307.800 -16.844 -22.045

-16.844	-222.937	-2.501
-22.045	-2.501	-86.726
258.884	-4.015	2.041
-4.015	261.443	-1.185
2.041	-1.185	221.963

orbtensor 29 C

-161.790	-72.828	-44.309
-72.828	-204.988	86.462
-44.309	86.462	-261.856
247.878	14.961	13.443
14.961	246.760	-5.417
13.443	-5.417	250.396

orbtensor 30 C

-159.192	72.554	-41.267
72.554	-203.215	-85.844
-41.267	-85.844	-264.319
247.919	-15.018	13.383
-15.018	246.721	5.423
13.383	5.423	250.383

orbtensor 31 C

-164.283	71.804	42.844
71.804	-205.446	85.400
42.844	85.400	-263.825
247.929	-15.014	-13.385
-15.014	246.720	-5.428
-13.385	-5.428	250.377

orbtensor 32 C

-163.529	-72.412	43.416
-72.412	-203.840	-85.222
43.416	-85.222	-263.521
247.878	14.959	-13.446
14.959	246.764	5.419
-13.446	5.419	250.393

orbtensor 33 C

-152.629	-75.853	-41.131
-75.853	-200.352	95.170
-41.131	95.170	-233.250
244.306	15.918	10.860
15.918	244.351	-8.477
10.860	-8.477	246.517

orbtensor 34 C

-153.337	75.921	-39.832
75.921	-202.195	-93.379
-39.832	-93.379	-230.594
244.322	-15.957	10.787
-15.957	244.283	8.491
10.787	8.491	246.553

orbtensor 35 C

-151.330	77.267	43.691
77.267	-199.994	92.263
43.691	92.263	-233.838
244.330	-15.954	-10.790
-15.954	244.281	-8.497
-10.790	-8.497	246.544

orbtensor 36 C

-147.408	-75.655	45.476
-75.655	-201.719	-96.994
45.476	-96.994	-231.543
244.307	15.916	-10.863

15.916 244.355 8.478
 -10.863 8.478 246.514

gtensor (ppt)

-0.176 0.000 0.000
 0.000 -0.176 0.000
 0.000 0.000 -0.167
 13.419 -0.198 -0.081
 -0.198 14.116 0.360
 -0.081 0.360 4.072

zfstensor (cm-1)

-0.301506 0.000696 0.000027
 0.000696 -0.344285 -0.000081
 0.000027 -0.000081 1.688028

averaging

A Average:5,6,7,8,13,14,15,16

B Average:1,2,3,4,25,26,27,28

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	1.0393	43.23367	-1263.09252	-3.15770	-1266.25023	-1223.01656
2	C	1.0387	43.68800	-1262.28233	-3.12983	-1265.41216	-1221.72416
3	C	1.0387	43.00567	-1262.28233	-3.17571	-1265.45804	-1222.45237
4	C	1.0393	42.92300	-1263.09252	-3.11379	-1266.20631	-1223.28331
5	C	0.8523	24.94900	-1035.83309	-12.89129	-1048.72438	-1023.77538
6	C	0.8480	26.77200	-1030.56683	-12.94523	-1043.51206	-1016.74006
7	C	0.8480	25.36533	-1030.56683	-13.06937	-1043.63620	-1018.27087
8	C	0.8520	24.63767	-1035.42799	-12.79490	-1048.22289	-1023.58523
9	C	0.2913	51.39133	-354.05480	2.39777	-351.65703	-300.26569
10	C	0.2917	50.26867	-354.45990	2.32307	-352.13683	-301.86816
11	C	0.2917	50.47500	-354.45990	2.27828	-352.18162	-301.70662
12	C	0.2913	52.10467	-354.05480	2.42244	-351.63236	-299.52769
13	C	0.8390	24.52133	-1019.62921	-12.87192	-1032.50113	-1007.97980
14	C	0.8367	24.82167	-1016.79353	-13.00123	-1029.79476	-1004.97310
15	C	0.8367	26.18800	-1016.79353	-13.04417	-1029.83771	-1003.64971
16	C	0.8393	26.24867	-1020.03431	-12.85022	-1032.88453	-1006.63586
17	C	-0.1770	31.53567	215.10652	-2.05887	213.04765	244.58332
18	C	-0.1773	30.83667	215.51162	-2.10292	213.40869	244.24536
19	C	-0.1773	29.06967	215.51162	-2.11495	213.39666	242.46633
20	C	-0.1770	28.89500	215.10652	-2.05441	213.05211	241.94711
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2080	38.02433	-252.78054	-1.72437	-254.50492	-216.48058
24	C	0.2070	37.13433	-251.56525	-1.70305	-253.26830	-216.13397
25	C	1.0147	41.11600	-1233.11534	-3.41791	-1236.53325	-1195.41725
26	C	1.0130	41.25800	-1231.08986	-3.42936	-1234.51921	-1193.26121
27	C	1.0130	42.47933	-1231.08986	-3.43874	-1234.52860	-1192.04926
28	C	1.0147	41.60900	-1233.11534	-3.41364	-1236.52898	-1194.91998
29	C	0.2003	38.80000	-243.46331	-1.20612	-244.66943	-205.86943
30	C	0.2003	39.43233	-243.46331	-1.20914	-244.67245	-205.24012
31	C	0.2003	37.15733	-243.46331	-1.22995	-244.69326	-207.53593
32	C	0.2003	38.04833	-243.46331	-1.19301	-244.65633	-206.60799
33	C	0.0063	49.64767	-7.69684	-0.75428	-8.45112	41.19655
34	C	0.0067	49.67733	-8.10194	-0.77863	-8.88057	40.79676
35	C	0.0067	49.99767	-8.10194	-0.77557	-8.87751	41.12016
36	C	0.0063	51.50200	-7.69684	-0.75767	-8.45451	43.04749
A Average		0.8440	25.43796	-1025.70567	-12.93354	-1038.63921	-1013.20125
B Average		1.0264	42.41408	-1247.39501	-3.28459	-1250.67960	-1208.26551
M Average		0.2915	51.05992	-354.25735	2.35539	-351.90196	-300.84204

=====
 FeL5-planar-HS-STO-PBE0-Full-ORCA

Temperature: 303
Spin: 2.5

atensor 1 C
0.755 0.070 0.015
0.070 1.541 0.154
0.015 0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C
0.754 -0.071 0.016
-0.071 1.540 -0.154
0.016 -0.154 0.830
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C
0.754 -0.071 -0.016
-0.071 1.540 0.154
-0.016 0.154 0.830
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.755 0.070 -0.015
0.070 1.541 -0.154
-0.015 -0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.746 0.807 0.148
0.807 1.849 0.397
0.148 0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 0.001
0.000 0.001 0.002

atensor 6 C
0.742 -0.808 0.144
-0.808 1.846 -0.394
0.144 -0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 7 C
0.743 -0.808 -0.144
-0.808 1.846 0.394
-0.144 0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 0.001
0.000 0.001 0.002

atensor 8 C
0.746 0.807 -0.148
0.807 1.849 -0.397
-0.148 -0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 9 C
0.210 0.590 0.152
0.590 0.210 0.119
0.152 0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 0.001
0.002 0.000 0.000

atensor 10 C
0.211 -0.591 0.153
-0.591 0.210 -0.119
0.153 -0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 -0.001
0.002 0.000 0.000

atensor 11 C
0.211 -0.591 -0.153
-0.591 0.210 0.119
-0.153 0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 0.001
-0.002 0.000 0.000

atensor 12 C
0.210 0.590 -0.152
0.590 0.210 -0.119
-0.152 -0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 -0.001
-0.002 0.000 0.000

atensor 13 C
1.880 0.825 0.244
0.825 0.723 0.098
0.244 0.098 -0.087
0.003 0.007 0.001
0.005 -0.002 0.000
0.001 -0.001 0.001

atensor 14 C
1.881 -0.825 0.240
-0.825 0.719 -0.094
0.240 -0.094 -0.091
0.003 -0.007 0.001
-0.005 -0.002 0.000
0.001 0.001 0.001

atensor 15 C
1.880 -0.825 -0.240
-0.825 0.719 0.094
-0.240 0.094 -0.091
0.003 -0.007 -0.001
-0.005 -0.002 0.000
-0.001 -0.001 0.001

atensor 16 C
1.880 0.825 -0.244
0.825 0.723 -0.098
-0.244 -0.098 -0.087
0.003 0.007 -0.001
0.004 -0.002 0.000
-0.001 0.001 0.001

atensor 17 C
-0.106 0.239 0.060
0.239 -0.103 0.029

0.060 0.029 -0.323
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.106 -0.239 0.059
-0.239 -0.103 -0.028
0.059 -0.028 -0.324
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.106 -0.239 -0.059
-0.239 -0.103 0.028
-0.059 0.028 -0.324
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.106 0.239 -0.060
0.239 -0.103 -0.029
-0.060 -0.029 -0.323
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.216 -0.135 0.019
-0.135 0.318 -0.011
0.019 -0.011 0.089
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.216 0.135 0.018
0.135 0.317 0.009
0.018 0.009 0.088
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.562 0.078 0.038
0.078 0.727 0.023
0.038 0.023 0.763
0.002 -0.001 0.001
0.000 -0.009 0.000
0.001 0.001 -0.001

atensor 26 C
1.561 -0.077 0.038
-0.077 0.725 -0.023
0.038 -0.023 0.761
0.002 0.001 0.001
0.000 -0.009 0.000
0.001 -0.001 -0.001

atensor 27 C
1.561 -0.077 -0.038
-0.077 0.725 0.023
-0.038 0.023 0.761
0.002 0.001 -0.001
0.000 -0.009 0.000

-0.001 0.001 -0.001

atensor 28 C

1.562 0.078 -0.038
0.078 0.727 -0.023
-0.038 -0.023 0.763
0.002 -0.001 -0.001
0.000 -0.009 0.000
-0.001 -0.001 -0.001

atensor 29 C

0.290 0.111 0.061
0.111 0.197 0.059
0.061 0.059 0.114
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C

0.290 -0.111 0.060
-0.111 0.197 -0.058
0.060 -0.058 0.114
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C

0.290 -0.111 -0.060
-0.111 0.197 0.058
-0.060 0.058 0.114
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C

0.290 0.111 -0.061
0.111 0.197 -0.059
-0.061 -0.059 0.114
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C

0.020 0.092 0.003
0.092 0.046 -0.011
0.003 -0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C

0.021 -0.092 0.002
-0.092 0.046 0.011
0.002 0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C

0.021 -0.092 -0.002
-0.092 0.046 -0.011
-0.002 -0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C

0.020 0.092 -0.003
0.092 0.046 0.011
-0.003 0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.035 0.082 0.037
0.082 0.015 0.020
0.037 0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.035 -0.082 0.037
-0.082 0.015 -0.019
0.037 -0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.035 -0.082 -0.037
-0.082 0.015 0.019
-0.037 0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.035 0.082 -0.037
0.082 0.015 -0.020
-0.037 -0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.041 0.046 -0.003
0.046 0.039 0.021
-0.003 0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.046 -0.003
-0.046 0.039 -0.021
-0.003 -0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.046 0.003
-0.046 0.039 0.021
0.003 0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.046 0.003
0.046 0.039 -0.021
0.003 -0.021 -0.028

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.116 0.407 0.085
0.407 1.135 0.297
0.085 0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 0.002
0.000 0.001 -0.001

atensor 48 H
-0.116 -0.408 0.084
-0.408 1.135 -0.295
0.084 -0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 49 H
-0.116 -0.408 -0.084
-0.408 1.135 0.295
-0.084 0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 0.002
0.000 0.001 -0.001

atensor 50 H
-0.116 0.407 -0.085
0.407 1.135 -0.297
-0.085 -0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 51 H
-0.073 0.628 -0.167
0.628 0.430 -0.263
-0.167 -0.263 -0.421
0.000 0.005 -0.001
0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 52 H
-0.073 -0.629 -0.170
-0.629 0.429 0.268
-0.170 0.268 -0.419
0.000 -0.005 -0.001
-0.005 0.003 0.001
0.000 0.000 -0.001

atensor 53 H
-0.073 -0.629 0.170
-0.629 0.429 -0.268
0.170 -0.268 -0.419
0.000 -0.005 0.001
-0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 54 H
-0.073 0.628 0.167
0.628 0.430 0.263
0.167 0.263 -0.421
0.000 0.005 0.001
0.005 0.003 0.001
0.000 0.000 -0.001

atensor 55 H
0.233 0.441 0.429
0.441 -0.126 0.276
0.429 0.276 -0.172
0.001 0.002 0.003
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.234 -0.443 0.427
-0.443 -0.124 -0.275
0.427 -0.275 -0.175
0.001 -0.002 0.003
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.234 -0.443 -0.427
-0.443 -0.124 0.275
-0.427 0.275 -0.175
0.001 -0.002 -0.003
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.233 0.441 -0.429
0.441 -0.126 -0.276
-0.429 -0.276 -0.172
0.001 0.002 -0.003
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.030 0.235 -0.038
0.235 0.155 -0.051
-0.038 -0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.030 -0.235 -0.039
-0.235 0.155 0.053
-0.039 0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.030 -0.235 0.039
-0.235 0.155 -0.053
0.039 -0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.030 0.235 0.038
0.235 0.155 0.051
0.038 0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.208 0.430 0.099

0.430 -0.136 0.031
0.099 0.031 -0.311
0.005 0.002 0.002
0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 64 H
1.208 -0.429 0.096
-0.429 -0.137 -0.030
0.096 -0.030 -0.312
0.005 -0.002 0.002
-0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 65 H
1.208 -0.429 -0.096
-0.429 -0.137 0.030
-0.096 0.030 -0.312
0.005 -0.002 -0.002
-0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 66 H
1.208 0.430 -0.099
0.430 -0.136 -0.031
-0.099 -0.031 -0.311
0.005 0.002 -0.002
0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 67 H
0.114 0.195 0.116
0.195 0.012 0.088
0.116 0.088 -0.085
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.114 -0.196 0.115
-0.196 0.013 -0.088
0.115 -0.088 -0.086
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.114 -0.196 -0.115
-0.196 0.013 0.088
-0.115 0.088 -0.086
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.114 0.195 -0.116
0.195 0.012 -0.088
-0.116 -0.088 -0.085
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.042 0.170 0.023
0.170 0.044 0.028
0.023 0.028 -0.130
0.000 0.001 0.000

0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.042 -0.170 0.022
-0.170 0.044 -0.027
0.022 -0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.042 -0.170 -0.022
-0.170 0.044 0.027
-0.022 0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.042 0.170 -0.023
0.170 0.044 -0.028
-0.023 -0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-222.856 -15.441 -1.797
-15.441 -302.054 -41.543
-1.797 -41.543 -87.648
261.510 -4.054 -0.922
-4.054 258.053 5.920
-0.922 5.920 222.696

orbtensor 2 C
-223.014 16.761 2.778
16.761 -299.984 41.884
2.778 41.884 -88.196
261.493 4.030 -1.127
4.030 258.060 -5.929
-1.127 -5.929 222.705

orbtensor 3 C
-223.132 16.202 -1.526
16.202 -300.516 -39.721
-1.526 -39.721 -89.594
261.493 4.030 1.125
4.030 258.060 5.931
1.125 5.931 222.706

orbtensor 4 C
-222.803 -16.997 0.252
-16.997 -301.519 44.429
0.252 44.429 -89.167
261.510 -4.053 0.920
-4.053 258.053 -5.918
0.920 -5.918 222.695

orbtensor 5 C
-283.518 -6.839 -2.496
-6.839 -297.188 -32.053
-2.496 -32.053 -109.849
270.694 2.204 0.455
2.204 265.836 4.951
0.455 4.951 228.872

orbtensor 6 C
-283.169 6.751 0.022
6.751 -293.464 34.072
0.022 34.072 -108.487
270.708 -2.227 0.285
-2.227 265.850 -4.902
0.285 -4.902 228.878

orbtensor 7 C
-281.417 5.524 2.548
5.524 -296.065 -33.489
2.548 -33.489 -111.853
270.706 -2.226 -0.286
-2.226 265.848 4.905
-0.286 4.905 228.877

orbtensor 8 C
-281.753 -6.301 0.116
-6.301 -296.147 33.055
0.116 33.055 -113.589
270.695 2.204 -0.457
2.204 265.836 -4.950
-0.457 -4.950 228.871

orbtensor 9 C
-256.114 -12.899 4.949
-12.899 -256.778 -21.424
4.949 -21.424 -75.935
262.817 0.522 0.776
0.522 262.852 2.900
0.776 2.900 217.332

orbtensor 10 C
-257.018 10.847 3.512
10.847 -258.260 20.675
3.512 20.675 -76.929
262.813 -0.536 0.627
-0.536 262.882 -2.748
0.627 -2.748 217.318

orbtensor 11 C
-258.134 12.197 -6.781
12.197 -257.286 -21.930
-6.781 -21.930 -76.167
262.814 -0.536 -0.628
-0.536 262.880 2.750
-0.628 2.750 217.318

orbtensor 12 C
-256.347 -11.281 -1.707
-11.281 -256.573 21.351
-1.707 21.351 -73.763
262.815 0.523 -0.778
0.523 262.852 -2.897
-0.778 -2.897 217.330

orbtensor 13 C
-298.065 -6.412 12.362
-6.412 -286.327 -3.750
12.362 -3.750 -107.790
266.304 2.067 -0.214
2.067 270.874 1.957
-0.214 1.957 228.568

orbtensor 14 C
-298.237 7.973 13.123
7.973 -284.550 3.905

13.123 3.905 -108.512
266.311 -2.065 -0.257
-2.065 270.892 -1.778
-0.257 -1.778 228.561

orbtensor 15 C
-299.216 7.653 -14.399
7.653 -283.915 -8.652
-14.399 -8.652 -104.072
266.312 -2.066 0.257
-2.066 270.892 1.781
0.257 1.781 228.563

orbtensor 16 C
-298.254 -5.534 -14.430
-5.534 -284.064 5.084
-14.430 5.084 -104.682
266.304 2.067 0.214
2.067 270.874 -1.954
0.214 -1.954 228.568

orbtensor 17 C
-217.551 -106.228 -56.647
-106.228 -227.046 47.957
-56.647 47.957 -217.887
252.329 14.873 10.149
14.873 254.103 -8.807
10.149 -8.807 250.659

orbtensor 18 C
-217.075 106.962 -55.380
106.962 -226.613 -48.087
-55.380 -48.087 -220.922
252.369 -14.901 10.063
-14.901 254.033 8.845
10.063 8.845 250.718

orbtensor 19 C
-220.287 107.565 57.620
107.565 -228.946 46.452
57.620 46.452 -220.680
252.374 -14.897 -10.067
-14.897 254.036 -8.849
-10.067 -8.849 250.712

orbtensor 20 C
-220.317 -108.397 55.496
-108.397 -228.227 -47.598
55.496 -47.598 -221.872
252.332 14.869 -10.151
14.869 254.109 8.809
-10.151 8.809 250.660

orbtensor 23 C
-189.408 69.892 85.922
69.892 -172.383 44.923
85.922 44.923 -269.970
245.741 -15.658 -6.123
-15.658 250.597 -12.110
-6.123 -12.110 249.496

orbtensor 24 C
-190.533 -70.911 85.463
-70.911 -171.824 -45.361
85.463 -45.361 -272.059
245.730 15.657 -6.199
15.657 250.691 12.075

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-6.199    12.075    249.398

orbtensor 25 C
-307.696  -16.097    21.744
-16.097  -225.894    7.542
21.744    7.542   -85.351
258.883   -4.015   -2.040
-4.015   261.443    1.187
-2.040    1.187   221.963

orbtensor 26 C
-309.811    13.676    22.442
13.676  -221.257   -4.335
22.442   -4.335  -87.456
258.886    4.025   -2.027
4.025   261.456   -0.975
-2.027   -0.975   221.956

orbtensor 27 C
-308.240    14.531   -23.321
14.531  -219.568    9.035
-23.321    9.035  -87.052
258.887    4.024    2.029
4.024   261.456    0.978
2.029    0.978   221.955

orbtensor 28 C
-307.800   -16.844   -22.045
-16.844  -222.937   -2.501
-22.045   -2.501  -86.726
258.884   -4.015    2.041
-4.015   261.443   -1.185
2.041   -1.185   221.963

orbtensor 29 C
-161.790   -72.828   -44.309
-72.828  -204.988    86.462
-44.309    86.462  -261.856
247.878   14.961   13.443
14.961   246.760   -5.417
13.443   -5.417   250.396

orbtensor 30 C
-159.192    72.554   -41.267
72.554  -203.215   -85.844
-41.267   -85.844  -264.319
247.919   -15.018   13.383
-15.018   246.721    5.423
13.383    5.423   250.383

orbtensor 31 C
-164.283    71.804    42.844
71.804  -205.446    85.400
42.844    85.400  -263.825
247.929   -15.014   -13.385
-15.014   246.720   -5.428
-13.385   -5.428   250.377

orbtensor 32 C
-163.529   -72.412    43.416
-72.412  -203.840   -85.222
43.416   -85.222  -263.521
247.878   14.959   -13.446
14.959   246.764    5.419
-13.446    5.419   250.393

orbtensor 33 C

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-152.629 -75.853 -41.131
-75.853 -200.352 95.170
-41.131 95.170 -233.250
244.306 15.918 10.860
15.918 244.351 -8.477
10.860 -8.477 246.517

orbtensor 34 C
-153.337 75.921 -39.832
75.921 -202.195 -93.379
-39.832 -93.379 -230.594
244.322 -15.957 10.787
-15.957 244.283 8.491
10.787 8.491 246.553

orbtensor 35 C
-151.330 77.267 43.691
77.267 -199.994 92.263
43.691 92.263 -233.838
244.330 -15.954 -10.790
-15.954 244.281 -8.497
-10.790 -8.497 246.544

orbtensor 36 C
-147.408 -75.655 45.476
-75.655 -201.719 -96.994
45.476 -96.994 -231.543
244.307 15.916 -10.863
15.916 244.355 8.478
-10.863 8.478 246.514

orbtensor 37 C
-184.308 -71.579 -96.166
-71.579 -157.953 42.683
-96.166 42.683 -240.461
242.769 16.007 9.554
16.007 246.572 -9.530
9.554 -9.530 246.313

orbtensor 38 C
-186.432 73.930 -95.546
73.930 -159.485 -41.347
-95.546 -41.347 -240.707
242.793 -16.032 9.485
-16.032 246.507 9.554
9.485 9.554 246.371

orbtensor 39 C
-186.961 72.882 98.050
72.882 -158.399 42.150
98.050 42.150 -239.645
242.801 -16.029 -9.488
-16.029 246.506 -9.560
-9.488 -9.560 246.363

orbtensor 40 C
-184.878 -73.069 96.556
-73.069 -160.540 -42.683
96.556 -42.683 -242.074
242.768 16.005 -9.557
16.005 246.575 9.531
-9.557 9.531 246.308

orbtensor 41 C
-196.270 -117.986 -57.600
-117.986 -207.488 46.829
-57.600 46.829 -184.913

243.818	12.812	10.677
12.812	245.851	-10.137
10.677	-10.137	250.681

orbtensor 42 C

-198.333	116.389	-56.673
116.389	-210.886	-46.776
-56.673	-46.776	-186.504
243.841	-12.844	10.631
-12.844	245.768	10.131
10.631	10.131	250.739

orbtensor 43 C

-197.668	118.936	57.375
118.936	-209.971	46.789
57.375	46.789	-183.741
243.849	-12.840	-10.634
-12.840	245.768	-10.137
-10.634	-10.137	250.730

orbtensor 44 C

-196.601	-117.647	57.945
-117.647	-210.663	-49.000
57.945	-49.000	-186.292
243.819	12.809	-10.680
12.809	245.854	10.138
-10.680	10.138	250.677

orbtensor 47 H

-3.449	-8.025	-1.380
-8.025	-15.587	-2.691
-1.380	-2.691	-5.092
35.460	4.745	-0.172
4.745	35.627	3.116
-0.172	3.116	18.711

orbtensor 48 H

-3.524	7.932	-1.571
7.932	-15.613	2.737
-1.571	2.737	-5.125
35.457	-4.755	-0.250
-4.755	35.626	-3.080
-0.250	-3.080	18.706

orbtensor 49 H

-3.429	7.924	1.298
7.924	-15.825	-2.619
1.298	-2.619	-4.804
35.456	-4.755	0.250
-4.755	35.626	3.082
0.250	3.082	18.706

orbtensor 50 H

-3.503	-7.956	1.704
-7.956	-15.697	2.894
1.704	2.894	-4.810
35.461	4.745	0.172
4.745	35.626	-3.116
0.172	-3.116	18.710

orbtensor 51 H

-8.548	-0.972	-9.078
-0.972	-3.572	-2.160
-9.078	-2.160	-16.494
31.287	4.573	5.532
4.573	27.487	-3.735
5.532	-3.735	34.496

orbtensor 52 H
-8.621 0.873 -8.930
0.873 -3.668 2.365
-8.930 2.365 -16.561
31.290 -4.598 5.519
-4.598 27.460 3.703
5.519 3.703 34.511

orbtensor 53 H
-8.688 0.664 8.816
0.664 -3.694 -2.451
8.816 -2.451 -16.551
31.294 -4.597 -5.520
-4.597 27.460 -3.706
-5.520 -3.706 34.506

orbtensor 54 H
-8.531 -0.841 9.044
-0.841 -3.667 2.424
9.044 2.424 -16.472
31.289 4.573 -5.532
4.573 27.488 3.736
-5.532 3.736 34.494

orbtensor 55 H
-3.571 -1.099 3.338
-1.099 -10.012 9.700
3.338 9.700 -14.591
26.832 4.401 3.615
4.401 32.581 -5.335
3.615 -5.335 34.284

orbtensor 56 H
-3.805 0.956 3.345
0.956 -9.968 -9.542
3.345 -9.542 -14.710
26.848 -4.400 3.615
-4.400 32.532 5.337
3.615 5.337 34.319

orbtensor 57 H
-3.852 0.858 -3.540
0.858 -10.175 9.510
-3.540 9.510 -14.702
26.850 -4.399 -3.617
-4.399 32.534 -5.338
-3.617 -5.338 34.316

orbtensor 58 H
-3.831 -0.835 -3.573
-0.835 -10.250 -9.460
-3.573 -9.460 -14.699
26.831 4.400 -3.617
4.400 32.583 5.336
-3.617 5.336 34.282

orbtensor 59 H
-1.057 -2.824 0.588
-2.824 -9.100 8.643
0.588 8.643 -11.960
26.917 4.379 0.302
4.379 33.312 -8.820
0.302 -8.820 33.689

orbtensor 60 H
-0.857 2.975 0.456

2.975	-8.731	-8.767
0.456	-8.767	-11.832
26.910	-4.358	0.298
-4.358	33.229	8.826
0.298	8.826	33.777

orbtensor 61 H

-0.775	3.192	-0.532
3.192	-8.567	8.940
-0.532	8.940	-11.581
26.911	-4.357	-0.300
-4.357	33.231	-8.827
-0.300	-8.827	33.773

orbtensor 62 H

-0.990	-3.119	-0.459
-3.119	-8.881	-8.996
-0.459	-8.996	-11.616
26.917	4.377	-0.305
4.377	33.314	8.821
-0.305	8.821	33.688

orbtensor 63 H

-16.081	-8.188	2.183
-8.188	-3.698	1.306
2.183	1.306	-4.684
36.175	4.783	-1.278
4.783	35.253	1.178
-1.278	1.178	18.423

orbtensor 64 H

-16.053	8.003	2.149
8.003	-3.776	-1.246
2.149	-1.246	-4.342
36.183	-4.777	-1.311
-4.777	35.259	-1.090
-1.311	-1.090	18.413

orbtensor 65 H

-16.299	7.959	-2.397
7.959	-3.548	1.290
-2.397	1.290	-4.701
36.183	-4.778	1.311
-4.778	35.260	1.091
1.311	1.091	18.413

orbtensor 66 H

-16.283	-8.089	-2.184
-8.089	-3.545	-1.260
-2.184	-1.260	-4.684
36.176	4.783	1.279
4.783	35.254	-1.177
1.279	-1.177	18.423

orbtensor 67 H

-7.725	-2.072	-8.240
-2.072	-1.305	0.096
-8.240	0.096	-13.178
31.850	3.758	8.935
3.758	27.157	-0.498
8.935	-0.498	35.029

orbtensor 68 H

-7.593	2.221	-8.512
2.221	-1.044	-0.151
-8.512	-0.151	-12.801
31.884	-3.806	8.924

```
-3.806 27.156 0.460
8.924 0.460 34.997
```

```
orbtensor 69 H
-7.302 2.401 8.589
2.401 -1.051 0.265
8.589 0.265 -12.952
31.889 -3.805 -8.925
-3.805 27.155 -0.463
-8.925 -0.463 34.992
```

```
orbtensor 70 H
-7.644 -2.124 8.411
-2.124 -1.117 -0.086
8.411 -0.086 -13.068
31.851 3.758 -8.936
3.758 27.157 0.499
-8.936 0.499 35.026
```

```
orbtensor 71 H
-8.801 -10.741 -1.794
-10.741 -9.317 0.495
-1.794 0.495 -2.211
33.480 9.739 2.342
9.739 34.042 -1.082
2.342 -1.082 26.828
```

```
orbtensor 72 H
-8.552 11.133 -2.028
11.133 -9.005 -0.865
-2.028 -0.865 -1.718
33.473 -9.749 2.278
-9.749 34.048 1.137
2.278 1.137 26.830
```

```
orbtensor 73 H
-8.356 11.370 2.206
11.370 -8.787 0.936
2.206 0.936 -1.875
33.477 -9.748 -2.278
-9.748 34.046 -1.139
-2.278 -1.139 26.828
```

```
orbtensor 74 H
-8.588 -11.065 1.969
-11.065 -9.008 -0.744
1.969 -0.744 -1.754
33.479 9.738 -2.342
9.738 34.044 1.083
-2.342 1.083 26.827
```

```
gtensor (ppt)
-0.176 0.000 0.000
0.000 -0.176 0.000
0.000 0.000 -0.167
13.419 -0.198 -0.081
-0.198 14.116 0.360
-0.081 0.360 4.072
```

```
zfstensor (cm-1)
-0.301506 0.000696 0.000027
0.000696 -0.344285 -0.000081
0.000027 -0.000081 1.688028
```

```
averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
```

M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	1.0397	43.23367	-1263.49762	-3.16224	-1266.65986	-1223.42620
2	C	1.0387	43.68800	-1262.28233	-3.12983	-1265.41216	-1221.72416
3	C	1.0387	43.00567	-1262.28233	-3.17571	-1265.45804	-1222.45237
4	C	1.0397	42.92300	-1263.49762	-3.11833	-1266.61595	-1223.69295
5	C	0.8523	24.94900	-1035.83309	-12.89129	-1048.72438	-1023.77538
6	C	0.8480	26.77200	-1030.56683	-12.94523	-1043.51206	-1016.74006
7	C	0.8483	25.36533	-1030.97193	-13.07391	-1044.04584	-1018.68050
8	C	0.8523	24.63767	-1035.83309	-12.78541	-1048.61850	-1023.98084
9	C	0.2913	51.39133	-354.05480	2.39777	-351.65703	-300.26569
10	C	0.2917	50.26867	-354.45990	2.32307	-352.13683	-301.86816
11	C	0.2917	50.47500	-354.45990	2.27828	-352.18162	-301.70662
12	C	0.2913	52.10467	-354.05480	2.42244	-351.63236	-299.52769
13	C	0.8393	24.52133	-1020.03431	-12.86243	-1032.89674	-1008.37541
14	C	0.8370	24.82167	-1017.19863	-13.00577	-1030.20440	-1005.38273
15	C	0.8367	26.18800	-1016.79353	-13.04417	-1029.83771	-1003.64971
16	C	0.8393	26.24867	-1020.03431	-12.85022	-1032.88453	-1006.63586
17	C	-0.1770	31.53567	215.10652	-2.05887	213.04765	244.58332
18	C	-0.1773	30.83667	215.51162	-2.10292	213.40869	244.24536
19	C	-0.1773	29.06967	215.51162	-2.11495	213.39666	242.46633
20	C	-0.1770	28.89500	215.10652	-2.05441	213.05211	241.94711
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2080	38.02433	-252.78054	-1.72437	-254.50492	-216.48058
24	C	0.2073	37.13433	-251.97035	-1.70759	-253.67794	-216.54360
25	C	1.0147	41.11600	-1233.11534	-3.41791	-1236.53325	-1195.41725
26	C	1.0130	41.25800	-1231.08986	-3.42936	-1234.51921	-1193.26121
27	C	1.0130	42.47933	-1231.08986	-3.43874	-1234.52860	-1192.04926
28	C	1.0147	41.60900	-1233.11534	-3.41364	-1236.52898	-1194.91998
29	C	0.2003	38.80000	-243.46331	-1.20612	-244.66943	-205.86943
30	C	0.2003	39.43233	-243.46331	-1.20914	-244.67245	-205.24012
31	C	0.2003	37.15733	-243.46331	-1.22995	-244.69326	-207.53593
32	C	0.2003	38.04833	-243.46331	-1.19301	-244.65633	-206.60799
33	C	0.0063	49.64767	-7.69684	-0.75428	-8.45112	41.19655
34	C	0.0067	49.67733	-8.10194	-0.77863	-8.88057	40.79676
35	C	0.0067	49.99767	-8.10194	-0.77557	-8.87751	41.12016
36	C	0.0063	51.50200	-7.69684	-0.75767	-8.45451	43.04749
A Average		0.8442	25.43796	-1025.90821	-12.93231	-1038.84052	-1013.40256
B Average		1.0265	42.41408	-1247.49629	-3.28572	-1250.78201	-1208.36792
M Average		0.2915	51.05992	-354.25735	2.35539	-351.90196	-300.84204

=====
FeL5-planar-HS-STO-PBE0-No-ZFS

atensor 1 C
0.755 0.070 0.015
0.070 1.541 0.154
0.015 0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 0.001
-0.001 0.000 -0.001

atensor 2 C
0.754 -0.071 0.016
-0.071 1.540 -0.154
0.016 -0.154 0.830
-0.009 0.001 0.000
0.000 0.002 -0.001
-0.001 0.000 -0.001

atensor 3 C
0.754 -0.071 -0.016

-0.071 1.540 0.154
-0.016 0.154 0.830
-0.009 0.001 0.000
0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.755 0.070 -0.015
0.070 1.541 -0.154
-0.015 -0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.746 0.807 0.148
0.807 1.849 0.397
0.148 0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 0.001
0.000 0.001 0.002

atensor 6 C
0.742 -0.808 0.144
-0.808 1.846 -0.394
0.144 -0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 7 C
0.743 -0.808 -0.144
-0.808 1.846 0.394
-0.144 0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 0.001
0.000 0.001 0.002

atensor 8 C
0.746 0.807 -0.148
0.807 1.849 -0.397
-0.148 -0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 9 C
0.210 0.590 0.152
0.590 0.210 0.119
0.152 0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 0.001
0.002 0.000 0.000

atensor 10 C
0.211 -0.591 0.153
-0.591 0.210 -0.119
0.153 -0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 -0.001
0.002 0.000 0.000

atensor 11 C
0.211 -0.591 -0.153
-0.591 0.210 0.119
-0.153 0.119 0.457
-0.001 0.002 0.000

0.003 -0.002 0.001
-0.002 0.000 0.000

atensor 12 C
0.210 0.590 -0.152
0.590 0.210 -0.119
-0.152 -0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 -0.001
-0.002 0.000 0.000

atensor 13 C
1.880 0.825 0.244
0.825 0.723 0.098
0.244 0.098 -0.087
0.003 0.007 0.001
0.005 -0.002 0.000
0.001 -0.001 0.001

atensor 14 C
1.881 -0.825 0.240
-0.825 0.719 -0.094
0.240 -0.094 -0.091
0.003 -0.007 0.001
-0.005 -0.002 0.000
0.001 0.001 0.001

atensor 15 C
1.880 -0.825 -0.240
-0.825 0.719 0.094
-0.240 0.094 -0.091
0.003 -0.007 -0.001
-0.005 -0.002 0.000
-0.001 -0.001 0.001

atensor 16 C
1.880 0.825 -0.244
0.825 0.723 -0.098
-0.244 -0.098 -0.087
0.003 0.007 -0.001
0.004 -0.002 0.000
-0.001 0.001 0.001

atensor 17 C
-0.106 0.239 0.060
0.239 -0.103 0.029
0.060 0.029 -0.323
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.106 -0.239 0.059
-0.239 -0.103 -0.028
0.059 -0.028 -0.324
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.106 -0.239 -0.059
-0.239 -0.103 0.028
-0.059 0.028 -0.324
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.106 0.239 -0.060
0.239 -0.103 -0.029
-0.060 -0.029 -0.323
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.216 -0.135 0.019
-0.135 0.318 -0.011
0.019 -0.011 0.089
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.216 0.135 0.018
0.135 0.317 0.009
0.018 0.009 0.088
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.562 0.078 0.038
0.078 0.727 0.023
0.038 0.023 0.763
0.002 -0.001 0.001
0.000 -0.009 0.000
0.001 0.001 -0.001

atensor 26 C
1.561 -0.077 0.038
-0.077 0.725 -0.023
0.038 -0.023 0.761
0.002 0.001 0.001
0.000 -0.009 0.000
0.001 -0.001 -0.001

atensor 27 C
1.561 -0.077 -0.038
-0.077 0.725 0.023
-0.038 0.023 0.761
0.002 0.001 -0.001
0.000 -0.009 0.000
-0.001 0.001 -0.001

atensor 28 C
1.562 0.078 -0.038
0.078 0.727 -0.023
-0.038 -0.023 0.763
0.002 -0.001 -0.001
0.000 -0.009 0.000
-0.001 -0.001 -0.001

atensor 29 C
0.290 0.111 0.061
0.111 0.197 0.059
0.061 0.059 0.114
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.290 -0.111 0.060
-0.111 0.197 -0.058

0.060 -0.058 0.114
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.290 -0.111 -0.060
-0.111 0.197 0.058
-0.060 0.058 0.114
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.290 0.111 -0.061
0.111 0.197 -0.059
-0.061 -0.059 0.114
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.020 0.092 0.003
0.092 0.046 -0.011
0.003 -0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.021 -0.092 0.002
-0.092 0.046 0.011
0.002 0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.021 -0.092 -0.002
-0.092 0.046 -0.011
-0.002 -0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.020 0.092 -0.003
0.092 0.046 0.011
-0.003 0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.035 0.082 0.037
0.082 0.015 0.020
0.037 0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.035 -0.082 0.037
-0.082 0.015 -0.019
0.037 -0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000

0.000 0.000 0.000

atensor 39 C
0.035 -0.082 -0.037
-0.082 0.015 0.019
-0.037 0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.035 0.082 -0.037
0.082 0.015 -0.020
-0.037 -0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.041 0.046 -0.003
0.046 0.039 0.021
-0.003 0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.046 -0.003
-0.046 0.039 -0.021
-0.003 -0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.046 0.003
-0.046 0.039 0.021
0.003 0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.046 0.003
0.046 0.039 -0.021
0.003 -0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.116 0.407 0.085
0.407 1.135 0.297
0.085 0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 0.002
0.000 0.001 -0.001

atensor 48 H
-0.116 -0.408 0.084
-0.408 1.135 -0.295
0.084 -0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 49 H

-0.116 -0.408 -0.084
-0.408 1.135 0.295
-0.084 0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 0.002
0.000 0.001 -0.001

atensor 50 H
-0.116 0.407 -0.085
0.407 1.135 -0.297
-0.085 -0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 51 H
-0.073 0.628 -0.167
0.628 0.430 -0.263
-0.167 -0.263 -0.421
0.000 0.005 -0.001
0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 52 H
-0.073 -0.629 -0.170
-0.629 0.429 0.268
-0.170 0.268 -0.419
0.000 -0.005 -0.001
-0.005 0.003 0.001
0.000 0.000 -0.001

atensor 53 H
-0.073 -0.629 0.170
-0.629 0.429 -0.268
0.170 -0.268 -0.419
0.000 -0.005 0.001
-0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 54 H
-0.073 0.628 0.167
0.628 0.430 0.263
0.167 0.263 -0.421
0.000 0.005 0.001
0.005 0.003 0.001
0.000 0.000 -0.001

atensor 55 H
0.233 0.441 0.429
0.441 -0.126 0.276
0.429 0.276 -0.172
0.001 0.002 0.003
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.234 -0.443 0.427
-0.443 -0.124 -0.275
0.427 -0.275 -0.175
0.001 -0.002 0.003
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.234 -0.443 -0.427
-0.443 -0.124 0.275
-0.427 0.275 -0.175

0.001 -0.002 -0.003
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.233 0.441 -0.429
0.441 -0.126 -0.276
-0.429 -0.276 -0.172
0.001 0.002 -0.003
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.030 0.235 -0.038
0.235 0.155 -0.051
-0.038 -0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.030 -0.235 -0.039
-0.235 0.155 0.053
-0.039 0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.030 -0.235 0.039
-0.235 0.155 -0.053
0.039 -0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.030 0.235 0.038
0.235 0.155 0.051
0.038 0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.208 0.430 0.099
0.430 -0.136 0.031
0.099 0.031 -0.311
0.005 0.002 0.002
0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 64 H
1.208 -0.429 0.096
-0.429 -0.137 -0.030
0.096 -0.030 -0.312
0.005 -0.002 0.002
-0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 65 H
1.208 -0.429 -0.096
-0.429 -0.137 0.030
-0.096 0.030 -0.312
0.005 -0.002 -0.002
-0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 66 H
1.208 0.430 -0.099
0.430 -0.136 -0.031
-0.099 -0.031 -0.311
0.005 0.002 -0.002
0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 67 H
0.114 0.195 0.116
0.195 0.012 0.088
0.116 0.088 -0.085
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.114 -0.196 0.115
-0.196 0.013 -0.088
0.115 -0.088 -0.086
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.114 -0.196 -0.115
-0.196 0.013 0.088
-0.115 0.088 -0.086
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.114 0.195 -0.116
0.195 0.012 -0.088
-0.116 -0.088 -0.085
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.042 0.170 0.023
0.170 0.044 0.028
0.023 0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.042 -0.170 0.022
-0.170 0.044 -0.027
0.022 -0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.042 -0.170 -0.022
-0.170 0.044 0.027
-0.022 0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.042 0.170 -0.023

0.170 0.044 -0.028
-0.023 -0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-222.856 -15.441 -1.797
-15.441 -302.054 -41.543
-1.797 -41.543 -87.648
261.510 -4.054 -0.922
-4.054 258.053 5.920
-0.922 5.920 222.696

orbtensor 2 C
-223.014 16.761 2.778
16.761 -299.984 41.884
2.778 41.884 -88.196
261.493 4.030 -1.127
4.030 258.060 -5.929
-1.127 -5.929 222.705

orbtensor 3 C
-223.132 16.202 -1.526
16.202 -300.516 -39.721
-1.526 -39.721 -89.594
261.493 4.030 1.125
4.030 258.060 5.931
1.125 5.931 222.706

orbtensor 4 C
-222.803 -16.997 0.252
-16.997 -301.519 44.429
0.252 44.429 -89.167
261.510 -4.053 0.920
-4.053 258.053 -5.918
0.920 -5.918 222.695

orbtensor 5 C
-283.518 -6.839 -2.496
-6.839 -297.188 -32.053
-2.496 -32.053 -109.849
270.694 2.204 0.455
2.204 265.836 4.951
0.455 4.951 228.872

orbtensor 6 C
-283.169 6.751 0.022
6.751 -293.464 34.072
0.022 34.072 -108.487
270.708 -2.227 0.285
-2.227 265.850 -4.902
0.285 -4.902 228.878

orbtensor 7 C
-281.417 5.524 2.548
5.524 -296.065 -33.489
2.548 -33.489 -111.853
270.706 -2.226 -0.286
-2.226 265.848 4.905
-0.286 4.905 228.877

orbtensor 8 C
-281.753 -6.301 0.116
-6.301 -296.147 33.055
0.116 33.055 -113.589
270.695 2.204 -0.457

2.204 265.836 -4.950
-0.457 -4.950 228.871

orbtensor 9 C
-256.114 -12.899 4.949
-12.899 -256.778 -21.424
4.949 -21.424 -75.935
262.817 0.522 0.776
0.522 262.852 2.900
0.776 2.900 217.332

orbtensor 10 C
-257.018 10.847 3.512
10.847 -258.260 20.675
3.512 20.675 -76.929
262.813 -0.536 0.627
-0.536 262.882 -2.748
0.627 -2.748 217.318

orbtensor 11 C
-258.134 12.197 -6.781
12.197 -257.286 -21.930
-6.781 -21.930 -76.167
262.814 -0.536 -0.628
-0.536 262.880 2.750
-0.628 2.750 217.318

orbtensor 12 C
-256.347 -11.281 -1.707
-11.281 -256.573 21.351
-1.707 21.351 -73.763
262.815 0.523 -0.778
0.523 262.852 -2.897
-0.778 -2.897 217.330

orbtensor 13 C
-298.065 -6.412 12.362
-6.412 -286.327 -3.750
12.362 -3.750 -107.790
266.304 2.067 -0.214
2.067 270.874 1.957
-0.214 1.957 228.568

orbtensor 14 C
-298.237 7.973 13.123
7.973 -284.550 3.905
13.123 3.905 -108.512
266.311 -2.065 -0.257
-2.065 270.892 -1.778
-0.257 -1.778 228.561

orbtensor 15 C
-299.216 7.653 -14.399
7.653 -283.915 -8.652
-14.399 -8.652 -104.072
266.312 -2.066 0.257
-2.066 270.892 1.781
0.257 1.781 228.563

orbtensor 16 C
-298.254 -5.534 -14.430
-5.534 -284.064 5.084
-14.430 5.084 -104.682
266.304 2.067 0.214
2.067 270.874 -1.954
0.214 -1.954 228.568

orbtensor 17 C
-217.551 -106.228 -56.647
-106.228 -227.046 47.957
-56.647 47.957 -217.887
252.329 14.873 10.149
14.873 254.103 -8.807
10.149 -8.807 250.659

orbtensor 18 C
-217.075 106.962 -55.380
106.962 -226.613 -48.087
-55.380 -48.087 -220.922
252.369 -14.901 10.063
-14.901 254.033 8.845
10.063 8.845 250.718

orbtensor 19 C
-220.287 107.565 57.620
107.565 -228.946 46.452
57.620 46.452 -220.680
252.374 -14.897 -10.067
-14.897 254.036 -8.849
-10.067 -8.849 250.712

orbtensor 20 C
-220.317 -108.397 55.496
-108.397 -228.227 -47.598
55.496 -47.598 -221.872
252.332 14.869 -10.151
14.869 254.109 8.809
-10.151 8.809 250.660

orbtensor 23 C
-189.408 69.892 85.922
69.892 -172.383 44.923
85.922 44.923 -269.970
245.741 -15.658 -6.123
-15.658 250.597 -12.110
-6.123 -12.110 249.496

orbtensor 24 C
-190.533 -70.911 85.463
-70.911 -171.824 -45.361
85.463 -45.361 -272.059
245.730 15.657 -6.199
15.657 250.691 12.075
-6.199 12.075 249.398

orbtensor 25 C
-307.696 -16.097 21.744
-16.097 -225.894 7.542
21.744 7.542 -85.351
258.883 -4.015 -2.040
-4.015 261.443 1.187
-2.040 1.187 221.963

orbtensor 26 C
-309.811 13.676 22.442
13.676 -221.257 -4.335
22.442 -4.335 -87.456
258.886 4.025 -2.027
4.025 261.456 -0.975
-2.027 -0.975 221.956

orbtensor 27 C
-308.240 14.531 -23.321
14.531 -219.568 9.035

-23.321	9.035	-87.052
258.887	4.024	2.029
4.024	261.456	0.978
2.029	0.978	221.955

orbtensor 28 C

-307.800	-16.844	-22.045
-16.844	-222.937	-2.501
-22.045	-2.501	-86.726
258.884	-4.015	2.041
-4.015	261.443	-1.185
2.041	-1.185	221.963

orbtensor 29 C

-161.790	-72.828	-44.309
-72.828	-204.988	86.462
-44.309	86.462	-261.856
247.878	14.961	13.443
14.961	246.760	-5.417
13.443	-5.417	250.396

orbtensor 30 C

-159.192	72.554	-41.267
72.554	-203.215	-85.844
-41.267	-85.844	-264.319
247.919	-15.018	13.383
-15.018	246.721	5.423
13.383	5.423	250.383

orbtensor 31 C

-164.283	71.804	42.844
71.804	-205.446	85.400
42.844	85.400	-263.825
247.929	-15.014	-13.385
-15.014	246.720	-5.428
-13.385	-5.428	250.377

orbtensor 32 C

-163.529	-72.412	43.416
-72.412	-203.840	-85.222
43.416	-85.222	-263.521
247.878	14.959	-13.446
14.959	246.764	5.419
-13.446	5.419	250.393

orbtensor 33 C

-152.629	-75.853	-41.131
-75.853	-200.352	95.170
-41.131	95.170	-233.250
244.306	15.918	10.860
15.918	244.351	-8.477
10.860	-8.477	246.517

orbtensor 34 C

-153.337	75.921	-39.832
75.921	-202.195	-93.379
-39.832	-93.379	-230.594
244.322	-15.957	10.787
-15.957	244.283	8.491
10.787	8.491	246.553

orbtensor 35 C

-151.330	77.267	43.691
77.267	-199.994	92.263
43.691	92.263	-233.838
244.330	-15.954	-10.790
-15.954	244.281	-8.497

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-10.790   -8.497   246.544

orbtensor 36 C
-147.408  -75.655   45.476
-75.655  -201.719  -96.994
45.476   -96.994 -231.543
244.307   15.916  -10.863
15.916   244.355   8.478
-10.863    8.478  246.514

orbtensor 37 C
-184.308  -71.579  -96.166
-71.579  -157.953  42.683
-96.166   42.683 -240.461
242.769   16.007   9.554
16.007   246.572  -9.530
9.554    -9.530  246.313

orbtensor 38 C
-186.432   73.930  -95.546
73.930  -159.485  -41.347
-95.546  -41.347 -240.707
242.793  -16.032   9.485
-16.032  246.507   9.554
9.485    9.554  246.371

orbtensor 39 C
-186.961   72.882   98.050
72.882  -158.399   42.150
98.050   42.150 -239.645
242.801  -16.029  -9.488
-16.029  246.506  -9.560
-9.488   -9.560  246.363

orbtensor 40 C
-184.878  -73.069   96.556
-73.069  -160.540  -42.683
96.556  -42.683 -242.074
242.768   16.005  -9.557
16.005   246.575   9.531
-9.557    9.531  246.308

orbtensor 41 C
-196.270  -117.986  -57.600
-117.986  -207.488   46.829
-57.600   46.829 -184.913
243.818   12.812   10.677
12.812   245.851  -10.137
10.677  -10.137  250.681

orbtensor 42 C
-198.333   116.389  -56.673
116.389  -210.886  -46.776
-56.673  -46.776 -186.504
243.841  -12.844   10.631
-12.844  245.768   10.131
10.631   10.131  250.739

orbtensor 43 C
-197.668   118.936   57.375
118.936  -209.971   46.789
57.375   46.789 -183.741
243.849  -12.840  -10.634
-12.840  245.768  -10.137
-10.634  -10.137  250.730

orbtensor 44 C

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-196.601	-117.647	57.945
-117.647	-210.663	-49.000
57.945	-49.000	-186.292
243.819	12.809	-10.680
12.809	245.854	10.138
-10.680	10.138	250.677

orbtensor 47 H

-3.449	-8.025	-1.380
-8.025	-15.587	-2.691
-1.380	-2.691	-5.092
35.460	4.745	-0.172
4.745	35.627	3.116
-0.172	3.116	18.711

orbtensor 48 H

-3.524	7.932	-1.571
7.932	-15.613	2.737
-1.571	2.737	-5.125
35.457	-4.755	-0.250
-4.755	35.626	-3.080
-0.250	-3.080	18.706

orbtensor 49 H

-3.429	7.924	1.298
7.924	-15.825	-2.619
1.298	-2.619	-4.804
35.456	-4.755	0.250
-4.755	35.626	3.082
0.250	3.082	18.706

orbtensor 50 H

-3.503	-7.956	1.704
-7.956	-15.697	2.894
1.704	2.894	-4.810
35.461	4.745	0.172
4.745	35.626	-3.116
0.172	-3.116	18.710

orbtensor 51 H

-8.548	-0.972	-9.078
-0.972	-3.572	-2.160
-9.078	-2.160	-16.494
31.287	4.573	5.532
4.573	27.487	-3.735
5.532	-3.735	34.496

orbtensor 52 H

-8.621	0.873	-8.930
0.873	-3.668	2.365
-8.930	2.365	-16.561
31.290	-4.598	5.519
-4.598	27.460	3.703
5.519	3.703	34.511

orbtensor 53 H

-8.688	0.664	8.816
0.664	-3.694	-2.451
8.816	-2.451	-16.551
31.294	-4.597	-5.520
-4.597	27.460	-3.706
-5.520	-3.706	34.506

orbtensor 54 H

-8.531	-0.841	9.044
-0.841	-3.667	2.424
9.044	2.424	-16.472

31.289	4.573	-5.532
4.573	27.488	3.736
-5.532	3.736	34.494

orbtensor 55 H

-3.571	-1.099	3.338
-1.099	-10.012	9.700
3.338	9.700	-14.591
26.832	4.401	3.615
4.401	32.581	-5.335
3.615	-5.335	34.284

orbtensor 56 H

-3.805	0.956	3.345
0.956	-9.968	-9.542
3.345	-9.542	-14.710
26.848	-4.400	3.615
-4.400	32.532	5.337
3.615	5.337	34.319

orbtensor 57 H

-3.852	0.858	-3.540
0.858	-10.175	9.510
-3.540	9.510	-14.702
26.850	-4.399	-3.617
-4.399	32.534	-5.338
-3.617	-5.338	34.316

orbtensor 58 H

-3.831	-0.835	-3.573
-0.835	-10.250	-9.460
-3.573	-9.460	-14.699
26.831	4.400	-3.617
4.400	32.583	5.336
-3.617	5.336	34.282

orbtensor 59 H

-1.057	-2.824	0.588
-2.824	-9.100	8.643
0.588	8.643	-11.960
26.917	4.379	0.302
4.379	33.312	-8.820
0.302	-8.820	33.689

orbtensor 60 H

-0.857	2.975	0.456
2.975	-8.731	-8.767
0.456	-8.767	-11.832
26.910	-4.358	0.298
-4.358	33.229	8.826
0.298	8.826	33.777

orbtensor 61 H

-0.775	3.192	-0.532
3.192	-8.567	8.940
-0.532	8.940	-11.581
26.911	-4.357	-0.300
-4.357	33.231	-8.827
-0.300	-8.827	33.773

orbtensor 62 H

-0.990	-3.119	-0.459
-3.119	-8.881	-8.996
-0.459	-8.996	-11.616
26.917	4.377	-0.305
4.377	33.314	8.821
-0.305	8.821	33.688

orbtensor 63 H
-16.081 -8.188 2.183
-8.188 -3.698 1.306
2.183 1.306 -4.684
36.175 4.783 -1.278
4.783 35.253 1.178
-1.278 1.178 18.423

orbtensor 64 H
-16.053 8.003 2.149
8.003 -3.776 -1.246
2.149 -1.246 -4.342
36.183 -4.777 -1.311
-4.777 35.259 -1.090
-1.311 -1.090 18.413

orbtensor 65 H
-16.299 7.959 -2.397
7.959 -3.548 1.290
-2.397 1.290 -4.701
36.183 -4.778 1.311
-4.778 35.260 1.091
1.311 1.091 18.413

orbtensor 66 H
-16.283 -8.089 -2.184
-8.089 -3.545 -1.260
-2.184 -1.260 -4.684
36.176 4.783 1.279
4.783 35.254 -1.177
1.279 -1.177 18.423

orbtensor 67 H
-7.725 -2.072 -8.240
-2.072 -1.305 0.096
-8.240 0.096 -13.178
31.850 3.758 8.935
3.758 27.157 -0.498
8.935 -0.498 35.029

orbtensor 68 H
-7.593 2.221 -8.512
2.221 -1.044 -0.151
-8.512 -0.151 -12.801
31.884 -3.806 8.924
-3.806 27.156 0.460
8.924 0.460 34.997

orbtensor 69 H
-7.302 2.401 8.589
2.401 -1.051 0.265
8.589 0.265 -12.952
31.889 -3.805 -8.925
-3.805 27.155 -0.463
-8.925 -0.463 34.992

orbtensor 70 H
-7.644 -2.124 8.411
-2.124 -1.117 -0.086
8.411 -0.086 -13.068
31.851 3.758 -8.936
3.758 27.157 0.499
-8.936 0.499 35.026

orbtensor 71 H
-8.801 -10.741 -1.794

-10.741	-9.317	0.495
-1.794	0.495	-2.211
33.480	9.739	2.342
9.739	34.042	-1.082
2.342	-1.082	26.828

orbtensor 72 H

-8.552	11.133	-2.028
11.133	-9.005	-0.865
-2.028	-0.865	-1.718
33.473	-9.749	2.278
-9.749	34.048	1.137
2.278	1.137	26.830

orbtensor 73 H

-8.356	11.370	2.206
11.370	-8.787	0.936
2.206	0.936	-1.875
33.477	-9.748	-2.278
-9.748	34.046	-1.139
-2.278	-1.139	26.828

orbtensor 74 H

-8.588	-11.065	1.969
-11.065	-9.008	-0.744
1.969	-0.744	-1.754
33.479	9.738	-2.342
9.738	34.044	1.083
-2.342	1.083	26.827

gtensor (ppt)

-0.176	0.000	0.000
0.000	-0.176	0.000
0.000	0.000	-0.167
13.419	-0.198	-0.081
-0.198	14.116	0.360
-0.081	0.360	4.072

averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12
FeL5-planar-HS-STO-PBE0-No-G
Temperature: 303
Spin: 2.5

atensor 1 C

0.755	0.070	0.015
0.070	1.541	0.154
0.015	0.154	0.831
-0.009	-0.001	0.000
0.000	0.002	0.001
-0.001	0.000	-0.001

atensor 2 C

0.754	-0.071	0.016
-0.071	1.540	-0.154
0.016	-0.154	0.830
-0.009	0.001	0.000
0.000	0.002	-0.001
-0.001	0.000	-0.001

atensor 3 C

0.754	-0.071	-0.016
-0.071	1.540	0.154
-0.016	0.154	0.830
-0.009	0.001	0.000

0.000 0.002 0.001
0.001 0.000 -0.001

atensor 4 C
0.755 0.070 -0.015
0.070 1.541 -0.154
-0.015 -0.154 0.831
-0.009 -0.001 0.000
0.000 0.002 -0.001
0.001 0.000 -0.001

atensor 5 C
0.746 0.807 0.148
0.807 1.849 0.397
0.148 0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 0.001
0.000 0.001 0.002

atensor 6 C
0.742 -0.808 0.144
-0.808 1.846 -0.394
0.144 -0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 7 C
0.743 -0.808 -0.144
-0.808 1.846 0.394
-0.144 0.394 -0.047
-0.003 -0.005 0.000
-0.006 0.004 0.001
0.000 0.001 0.002

atensor 8 C
0.746 0.807 -0.148
0.807 1.849 -0.397
-0.148 -0.397 -0.041
-0.003 0.005 0.000
0.006 0.004 -0.001
0.000 -0.001 0.002

atensor 9 C
0.210 0.590 0.152
0.590 0.210 0.119
0.152 0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 0.001
0.002 0.000 0.000

atensor 10 C
0.211 -0.591 0.153
-0.591 0.210 -0.119
0.153 -0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 -0.001
0.002 0.000 0.000

atensor 11 C
0.211 -0.591 -0.153
-0.591 0.210 0.119
-0.153 0.119 0.457
-0.001 0.002 0.000
0.003 -0.002 0.001
-0.002 0.000 0.000

atensor 12 C
0.210 0.590 -0.152
0.590 0.210 -0.119
-0.152 -0.119 0.457
-0.001 -0.002 0.000
-0.003 -0.002 -0.001
-0.002 0.000 0.000

atensor 13 C
1.880 0.825 0.244
0.825 0.723 0.098
0.244 0.098 -0.087
0.003 0.007 0.001
0.005 -0.002 0.000
0.001 -0.001 0.001

atensor 14 C
1.881 -0.825 0.240
-0.825 0.719 -0.094
0.240 -0.094 -0.091
0.003 -0.007 0.001
-0.005 -0.002 0.000
0.001 0.001 0.001

atensor 15 C
1.880 -0.825 -0.240
-0.825 0.719 0.094
-0.240 0.094 -0.091
0.003 -0.007 -0.001
-0.005 -0.002 0.000
-0.001 -0.001 0.001

atensor 16 C
1.880 0.825 -0.244
0.825 0.723 -0.098
-0.244 -0.098 -0.087
0.003 0.007 -0.001
0.004 -0.002 0.000
-0.001 0.001 0.001

atensor 17 C
-0.106 0.239 0.060
0.239 -0.103 0.029
0.060 0.029 -0.323
0.001 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.106 -0.239 0.059
-0.239 -0.103 -0.028
0.059 -0.028 -0.324
0.001 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.106 -0.239 -0.059
-0.239 -0.103 0.028
-0.059 0.028 -0.324
0.001 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.106 0.239 -0.060
0.239 -0.103 -0.029

-0.060 -0.029 -0.323
0.001 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.216 -0.135 0.019
-0.135 0.318 -0.011
0.019 -0.011 0.089
0.000 -0.001 0.000
-0.001 0.001 0.000
0.000 0.000 0.000

atensor 24 C
0.216 0.135 0.018
0.135 0.317 0.009
0.018 0.009 0.088
0.000 0.001 0.000
0.001 0.001 0.000
0.000 0.000 0.000

atensor 25 C
1.562 0.078 0.038
0.078 0.727 0.023
0.038 0.023 0.763
0.002 -0.001 0.001
0.000 -0.009 0.000
0.001 0.001 -0.001

atensor 26 C
1.561 -0.077 0.038
-0.077 0.725 -0.023
0.038 -0.023 0.761
0.002 0.001 0.001
0.000 -0.009 0.000
0.001 -0.001 -0.001

atensor 27 C
1.561 -0.077 -0.038
-0.077 0.725 0.023
-0.038 0.023 0.761
0.002 0.001 -0.001
0.000 -0.009 0.000
-0.001 0.001 -0.001

atensor 28 C
1.562 0.078 -0.038
0.078 0.727 -0.023
-0.038 -0.023 0.763
0.002 -0.001 -0.001
0.000 -0.009 0.000
-0.001 -0.001 -0.001

atensor 29 C
0.290 0.111 0.061
0.111 0.197 0.059
0.061 0.059 0.114
0.000 0.001 0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.290 -0.111 0.060
-0.111 0.197 -0.058
0.060 -0.058 0.114
0.000 -0.001 0.001
-0.001 0.000 0.000

0.000 0.000 0.000

atensor 31 C
0.290 -0.111 -0.060
-0.111 0.197 0.058
-0.060 0.058 0.114
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.290 0.111 -0.061
0.111 0.197 -0.059
-0.061 -0.059 0.114
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.020 0.092 0.003
0.092 0.046 -0.011
0.003 -0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.021 -0.092 0.002
-0.092 0.046 0.011
0.002 0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.021 -0.092 -0.002
-0.092 0.046 -0.011
-0.002 -0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.020 0.092 -0.003
0.092 0.046 0.011
-0.003 0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.035 0.082 0.037
0.082 0.015 0.020
0.037 0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.035 -0.082 0.037
-0.082 0.015 -0.019
0.037 -0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 39 C

0.035 -0.082 -0.037
-0.082 0.015 0.019
-0.037 0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.035 0.082 -0.037
0.082 0.015 -0.020
-0.037 -0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.041 0.046 -0.003
0.046 0.039 0.021
-0.003 0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.046 -0.003
-0.046 0.039 -0.021
-0.003 -0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.046 0.003
-0.046 0.039 0.021
0.003 0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.046 0.003
0.046 0.039 -0.021
0.003 -0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.116 0.407 0.085
0.407 1.135 0.297
0.085 0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 0.002
0.000 0.001 -0.001

atensor 48 H
-0.116 -0.408 0.084
-0.408 1.135 -0.295
0.084 -0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 49 H
-0.116 -0.408 -0.084
-0.408 1.135 0.295
-0.084 0.295 -0.239

-0.004 -0.001 0.000
-0.002 0.005 0.002
0.000 0.001 -0.001

atensor 50 H
-0.116 0.407 -0.085
0.407 1.135 -0.297
-0.085 -0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 51 H
-0.073 0.628 -0.167
0.628 0.430 -0.263
-0.167 -0.263 -0.421
0.000 0.005 -0.001
0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 52 H
-0.073 -0.629 -0.170
-0.629 0.429 0.268
-0.170 0.268 -0.419
0.000 -0.005 -0.001
-0.005 0.003 0.001
0.000 0.000 -0.001

atensor 53 H
-0.073 -0.629 0.170
-0.629 0.429 -0.268
0.170 -0.268 -0.419
0.000 -0.005 0.001
-0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 54 H
-0.073 0.628 0.167
0.628 0.430 0.263
0.167 0.263 -0.421
0.000 0.005 0.001
0.005 0.003 0.001
0.000 0.000 -0.001

atensor 55 H
0.233 0.441 0.429
0.441 -0.126 0.276
0.429 0.276 -0.172
0.001 0.002 0.003
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.234 -0.443 0.427
-0.443 -0.124 -0.275
0.427 -0.275 -0.175
0.001 -0.002 0.003
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.234 -0.443 -0.427
-0.443 -0.124 0.275
-0.427 0.275 -0.175
0.001 -0.002 -0.003
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.233 0.441 -0.429
0.441 -0.126 -0.276
-0.429 -0.276 -0.172
0.001 0.002 -0.003
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.030 0.235 -0.038
0.235 0.155 -0.051
-0.038 -0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.030 -0.235 -0.039
-0.235 0.155 0.053
-0.039 0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 61 H
0.030 -0.235 0.039
-0.235 0.155 -0.053
0.039 -0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.030 0.235 0.038
0.235 0.155 0.051
0.038 0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.208 0.430 0.099
0.430 -0.136 0.031
0.099 0.031 -0.311
0.005 0.002 0.002
0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 64 H
1.208 -0.429 0.096
-0.429 -0.137 -0.030
0.096 -0.030 -0.312
0.005 -0.002 0.002
-0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 65 H
1.208 -0.429 -0.096
-0.429 -0.137 0.030
-0.096 0.030 -0.312
0.005 -0.002 -0.002
-0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 66 H
1.208 0.430 -0.099

0.430 -0.136 -0.031
-0.099 -0.031 -0.311
0.005 0.002 -0.002
0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 67 H
0.114 0.195 0.116
0.195 0.012 0.088
0.116 0.088 -0.085
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.114 -0.196 0.115
-0.196 0.013 -0.088
0.115 -0.088 -0.086
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H
0.114 -0.196 -0.115
-0.196 0.013 0.088
-0.115 0.088 -0.086
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.114 0.195 -0.116
0.195 0.012 -0.088
-0.116 -0.088 -0.085
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.042 0.170 0.023
0.170 0.044 0.028
0.023 0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.042 -0.170 0.022
-0.170 0.044 -0.027
0.022 -0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.042 -0.170 -0.022
-0.170 0.044 0.027
-0.022 0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.042 0.170 -0.023
0.170 0.044 -0.028
-0.023 -0.028 -0.130
0.000 0.001 0.000

0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-222.856 -15.441 -1.797
-15.441 -302.054 -41.543
-1.797 -41.543 -87.648
261.510 -4.054 -0.922
-4.054 258.053 5.920
-0.922 5.920 222.696

orbtensor 2 C
-223.014 16.761 2.778
16.761 -299.984 41.884
2.778 41.884 -88.196
261.493 4.030 -1.127
4.030 258.060 -5.929
-1.127 -5.929 222.705

orbtensor 3 C
-223.132 16.202 -1.526
16.202 -300.516 -39.721
-1.526 -39.721 -89.594
261.493 4.030 1.125
4.030 258.060 5.931
1.125 5.931 222.706

orbtensor 4 C
-222.803 -16.997 0.252
-16.997 -301.519 44.429
0.252 44.429 -89.167
261.510 -4.053 0.920
-4.053 258.053 -5.918
0.920 -5.918 222.695

orbtensor 5 C
-283.518 -6.839 -2.496
-6.839 -297.188 -32.053
-2.496 -32.053 -109.849
270.694 2.204 0.455
2.204 265.836 4.951
0.455 4.951 228.872

orbtensor 6 C
-283.169 6.751 0.022
6.751 -293.464 34.072
0.022 34.072 -108.487
270.708 -2.227 0.285
-2.227 265.850 -4.902
0.285 -4.902 228.878

orbtensor 7 C
-281.417 5.524 2.548
5.524 -296.065 -33.489
2.548 -33.489 -111.853
270.706 -2.226 -0.286
-2.226 265.848 4.905
-0.286 4.905 228.877

orbtensor 8 C
-281.753 -6.301 0.116
-6.301 -296.147 33.055
0.116 33.055 -113.589
270.695 2.204 -0.457
2.204 265.836 -4.950
-0.457 -4.950 228.871

orbtensor 9 C
-256.114 -12.899 4.949
-12.899 -256.778 -21.424
4.949 -21.424 -75.935
262.817 0.522 0.776
0.522 262.852 2.900
0.776 2.900 217.332

orbtensor 10 C
-257.018 10.847 3.512
10.847 -258.260 20.675
3.512 20.675 -76.929
262.813 -0.536 0.627
-0.536 262.882 -2.748
0.627 -2.748 217.318

orbtensor 11 C
-258.134 12.197 -6.781
12.197 -257.286 -21.930
-6.781 -21.930 -76.167
262.814 -0.536 -0.628
-0.536 262.880 2.750
-0.628 2.750 217.318

orbtensor 12 C
-256.347 -11.281 -1.707
-11.281 -256.573 21.351
-1.707 21.351 -73.763
262.815 0.523 -0.778
0.523 262.852 -2.897
-0.778 -2.897 217.330

orbtensor 13 C
-298.065 -6.412 12.362
-6.412 -286.327 -3.750
12.362 -3.750 -107.790
266.304 2.067 -0.214
2.067 270.874 1.957
-0.214 1.957 228.568

orbtensor 14 C
-298.237 7.973 13.123
7.973 -284.550 3.905
13.123 3.905 -108.512
266.311 -2.065 -0.257
-2.065 270.892 -1.778
-0.257 -1.778 228.561

orbtensor 15 C
-299.216 7.653 -14.399
7.653 -283.915 -8.652
-14.399 -8.652 -104.072
266.312 -2.066 0.257
-2.066 270.892 1.781
0.257 1.781 228.563

orbtensor 16 C
-298.254 -5.534 -14.430
-5.534 -284.064 5.084
-14.430 5.084 -104.682
266.304 2.067 0.214
2.067 270.874 -1.954
0.214 -1.954 228.568

orbtensor 17 C
-217.551 -106.228 -56.647
-106.228 -227.046 47.957

-56.647	47.957	-217.887
252.329	14.873	10.149
14.873	254.103	-8.807
10.149	-8.807	250.659

orbtensor 18 C

-217.075	106.962	-55.380
106.962	-226.613	-48.087
-55.380	-48.087	-220.922
252.369	-14.901	10.063
-14.901	254.033	8.845
10.063	8.845	250.718

orbtensor 19 C

-220.287	107.565	57.620
107.565	-228.946	46.452
57.620	46.452	-220.680
252.374	-14.897	-10.067
-14.897	254.036	-8.849
-10.067	-8.849	250.712

orbtensor 20 C

-220.317	-108.397	55.496
-108.397	-228.227	-47.598
55.496	-47.598	-221.872
252.332	14.869	-10.151
14.869	254.109	8.809
-10.151	8.809	250.660

orbtensor 23 C

-189.408	69.892	85.922
69.892	-172.383	44.923
85.922	44.923	-269.970
245.741	-15.658	-6.123
-15.658	250.597	-12.110
-6.123	-12.110	249.496

orbtensor 24 C

-190.533	-70.911	85.463
-70.911	-171.824	-45.361
85.463	-45.361	-272.059
245.730	15.657	-6.199
15.657	250.691	12.075
-6.199	12.075	249.398

orbtensor 25 C

-307.696	-16.097	21.744
-16.097	-225.894	7.542
21.744	7.542	-85.351
258.883	-4.015	-2.040
-4.015	261.443	1.187
-2.040	1.187	221.963

orbtensor 26 C

-309.811	13.676	22.442
13.676	-221.257	-4.335
22.442	-4.335	-87.456
258.886	4.025	-2.027
4.025	261.456	-0.975
-2.027	-0.975	221.956

orbtensor 27 C

-308.240	14.531	-23.321
14.531	-219.568	9.035
-23.321	9.035	-87.052
258.887	4.024	2.029
4.024	261.456	0.978

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2.029      0.978    221.955

orbtensor 28 C
-307.800   -16.844   -22.045
-16.844   -222.937   -2.501
-22.045    -2.501   -86.726
258.884    -4.015    2.041
-4.015    261.443   -1.185
2.041     -1.185   221.963

orbtensor 29 C
-161.790   -72.828   -44.309
-72.828   -204.988   86.462
-44.309    86.462  -261.856
247.878    14.961   13.443
14.961    246.760   -5.417
13.443    -5.417   250.396

orbtensor 30 C
-159.192    72.554   -41.267
72.554   -203.215   -85.844
-41.267   -85.844  -264.319
247.919   -15.018   13.383
-15.018   246.721    5.423
13.383    5.423   250.383

orbtensor 31 C
-164.283    71.804    42.844
71.804   -205.446    85.400
42.844    85.400  -263.825
247.929   -15.014   -13.385
-15.014   246.720   -5.428
-13.385   -5.428   250.377

orbtensor 32 C
-163.529   -72.412    43.416
-72.412   -203.840   -85.222
43.416   -85.222  -263.521
247.878    14.959   -13.446
14.959    246.764    5.419
-13.446    5.419   250.393

orbtensor 33 C
-152.629   -75.853   -41.131
-75.853   -200.352    95.170
-41.131    95.170  -233.250
244.306    15.918    10.860
15.918    244.351   -8.477
10.860    -8.477   246.517

orbtensor 34 C
-153.337    75.921   -39.832
75.921   -202.195   -93.379
-39.832   -93.379  -230.594
244.322   -15.957    10.787
-15.957   244.283    8.491
10.787    8.491   246.553

orbtensor 35 C
-151.330    77.267    43.691
77.267   -199.994    92.263
43.691    92.263  -233.838
244.330   -15.954   -10.790
-15.954   244.281   -8.497
-10.790   -8.497   246.544

orbtensor 36 C

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-147.408 -75.655 45.476
-75.655 -201.719 -96.994
45.476 -96.994 -231.543
244.307 15.916 -10.863
15.916 244.355 8.478
-10.863 8.478 246.514

orbtensor 37 C
-184.308 -71.579 -96.166
-71.579 -157.953 42.683
-96.166 42.683 -240.461
242.769 16.007 9.554
16.007 246.572 -9.530
9.554 -9.530 246.313

orbtensor 38 C
-186.432 73.930 -95.546
73.930 -159.485 -41.347
-95.546 -41.347 -240.707
242.793 -16.032 9.485
-16.032 246.507 9.554
9.485 9.554 246.371

orbtensor 39 C
-186.961 72.882 98.050
72.882 -158.399 42.150
98.050 42.150 -239.645
242.801 -16.029 -9.488
-16.029 246.506 -9.560
-9.488 -9.560 246.363

orbtensor 40 C
-184.878 -73.069 96.556
-73.069 -160.540 -42.683
96.556 -42.683 -242.074
242.768 16.005 -9.557
16.005 246.575 9.531
-9.557 9.531 246.308

orbtensor 41 C
-196.270 -117.986 -57.600
-117.986 -207.488 46.829
-57.600 46.829 -184.913
243.818 12.812 10.677
12.812 245.851 -10.137
10.677 -10.137 250.681

orbtensor 42 C
-198.333 116.389 -56.673
116.389 -210.886 -46.776
-56.673 -46.776 -186.504
243.841 -12.844 10.631
-12.844 245.768 10.131
10.631 10.131 250.739

orbtensor 43 C
-197.668 118.936 57.375
118.936 -209.971 46.789
57.375 46.789 -183.741
243.849 -12.840 -10.634
-12.840 245.768 -10.137
-10.634 -10.137 250.730

orbtensor 44 C
-196.601 -117.647 57.945
-117.647 -210.663 -49.000
57.945 -49.000 -186.292

243.819	12.809	-10.680
12.809	245.854	10.138
-10.680	10.138	250.677

orbtensor 47 H

-3.449	-8.025	-1.380
-8.025	-15.587	-2.691
-1.380	-2.691	-5.092
35.460	4.745	-0.172
4.745	35.627	3.116
-0.172	3.116	18.711

orbtensor 48 H

-3.524	7.932	-1.571
7.932	-15.613	2.737
-1.571	2.737	-5.125
35.457	-4.755	-0.250
-4.755	35.626	-3.080
-0.250	-3.080	18.706

orbtensor 49 H

-3.429	7.924	1.298
7.924	-15.825	-2.619
1.298	-2.619	-4.804
35.456	-4.755	0.250
-4.755	35.626	3.082
0.250	3.082	18.706

orbtensor 50 H

-3.503	-7.956	1.704
-7.956	-15.697	2.894
1.704	2.894	-4.810
35.461	4.745	0.172
4.745	35.626	-3.116
0.172	-3.116	18.710

orbtensor 51 H

-8.548	-0.972	-9.078
-0.972	-3.572	-2.160
-9.078	-2.160	-16.494
31.287	4.573	5.532
4.573	27.487	-3.735
5.532	-3.735	34.496

orbtensor 52 H

-8.621	0.873	-8.930
0.873	-3.668	2.365
-8.930	2.365	-16.561
31.290	-4.598	5.519
-4.598	27.460	3.703
5.519	3.703	34.511

orbtensor 53 H

-8.688	0.664	8.816
0.664	-3.694	-2.451
8.816	-2.451	-16.551
31.294	-4.597	-5.520
-4.597	27.460	-3.706
-5.520	-3.706	34.506

orbtensor 54 H

-8.531	-0.841	9.044
-0.841	-3.667	2.424
9.044	2.424	-16.472
31.289	4.573	-5.532
4.573	27.488	3.736
-5.532	3.736	34.494

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orbtensor 55 H
-3.571   -1.099    3.338
-1.099  -10.012    9.700
3.338    9.700   -14.591
26.832   4.401    3.615
4.401   32.581   -5.335
3.615   -5.335   34.284

orbtensor 56 H
-3.805    0.956    3.345
0.956   -9.968   -9.542
3.345   -9.542  -14.710
26.848   -4.400    3.615
-4.400   32.532    5.337
3.615    5.337   34.319

orbtensor 57 H
-3.852    0.858   -3.540
0.858  -10.175    9.510
-3.540   9.510  -14.702
26.850   -4.399   -3.617
-4.399   32.534   -5.338
-3.617   -5.338   34.316

orbtensor 58 H
-3.831   -0.835   -3.573
-0.835  -10.250   -9.460
-3.573   -9.460  -14.699
26.831   4.400   -3.617
4.400   32.583    5.336
-3.617    5.336   34.282

orbtensor 59 H
-1.057   -2.824    0.588
-2.824   -9.100    8.643
0.588    8.643  -11.960
26.917   4.379    0.302
4.379   33.312   -8.820
0.302   -8.820   33.689

orbtensor 60 H
-0.857    2.975    0.456
2.975   -8.731   -8.767
0.456   -8.767  -11.832
26.910   -4.358    0.298
-4.358   33.229    8.826
0.298    8.826   33.777

orbtensor 61 H
-0.775    3.192   -0.532
3.192   -8.567    8.940
-0.532    8.940  -11.581
26.911   -4.357   -0.300
-4.357   33.231   -8.827
-0.300   -8.827   33.773

orbtensor 62 H
-0.990   -3.119   -0.459
-3.119   -8.881   -8.996
-0.459   -8.996  -11.616
26.917   4.377   -0.305
4.377   33.314    8.821
-0.305    8.821   33.688

orbtensor 63 H
-16.081   -8.188    2.183

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-8.188	-3.698	1.306
2.183	1.306	-4.684
36.175	4.783	-1.278
4.783	35.253	1.178
-1.278	1.178	18.423

orbtensor 64 H

-16.053	8.003	2.149
8.003	-3.776	-1.246
2.149	-1.246	-4.342
36.183	-4.777	-1.311
-4.777	35.259	-1.090
-1.311	-1.090	18.413

orbtensor 65 H

-16.299	7.959	-2.397
7.959	-3.548	1.290
-2.397	1.290	-4.701
36.183	-4.778	1.311
-4.778	35.260	1.091
1.311	1.091	18.413

orbtensor 66 H

-16.283	-8.089	-2.184
-8.089	-3.545	-1.260
-2.184	-1.260	-4.684
36.176	4.783	1.279
4.783	35.254	-1.177
1.279	-1.177	18.423

orbtensor 67 H

-7.725	-2.072	-8.240
-2.072	-1.305	0.096
-8.240	0.096	-13.178
31.850	3.758	8.935
3.758	27.157	-0.498
8.935	-0.498	35.029

orbtensor 68 H

-7.593	2.221	-8.512
2.221	-1.044	-0.151
-8.512	-0.151	-12.801
31.884	-3.806	8.924
-3.806	27.156	0.460
8.924	0.460	34.997

orbtensor 69 H

-7.302	2.401	8.589
2.401	-1.051	0.265
8.589	0.265	-12.952
31.889	-3.805	-8.925
-3.805	27.155	-0.463
-8.925	-0.463	34.992

orbtensor 70 H

-7.644	-2.124	8.411
-2.124	-1.117	-0.086
8.411	-0.086	-13.068
31.851	3.758	-8.936
3.758	27.157	0.499
-8.936	0.499	35.026

orbtensor 71 H

-8.801	-10.741	-1.794
-10.741	-9.317	0.495
-1.794	0.495	-2.211
33.480	9.739	2.342

9.739 34.042 -1.082
 2.342 -1.082 26.828

orbtensor 72 H
 -8.552 11.133 -2.028
 11.133 -9.005 -0.865
 -2.028 -0.865 -1.718
 33.473 -9.749 2.278
 -9.749 34.048 1.137
 2.278 1.137 26.830

orbtensor 73 H
 -8.356 11.370 2.206
 11.370 -8.787 0.936
 2.206 0.936 -1.875
 33.477 -9.748 -2.278
 -9.748 34.046 -1.139
 -2.278 -1.139 26.828

orbtensor 74 H
 -8.588 -11.065 1.969
 -11.065 -9.008 -0.744
 1.969 -0.744 -1.754
 33.479 9.738 -2.342
 9.738 34.044 1.083
 -2.342 1.083 26.827

gtensor (ppt)
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

averaging
 A Average:5,6,7,8,13,14,15,16
 B Average:1,2,3,4,25,26,27,28
 M Average:9,10,11,12

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	1.0397	43.23367	-1256.99197	0.00000	-1256.99197	-1213.75830
2	C	1.0387	43.68800	-1255.78294	0.00000	-1255.78294	-1212.09494
3	C	1.0387	43.00567	-1255.78294	0.00000	-1255.78294	-1212.77727
4	C	1.0397	42.92300	-1256.99197	0.00000	-1256.99197	-1214.06897
5	C	0.8523	24.94900	-1030.49967	-0.00000	-1030.49967	-1005.55067
6	C	0.8480	26.77200	-1025.26052	-0.00000	-1025.26052	-998.48852
7	C	0.8483	25.36533	-1025.66354	-0.00000	-1025.66354	-1000.29820
8	C	0.8523	24.63767	-1030.49967	-0.00000	-1030.49967	-1005.86200
9	C	0.2913	51.39133	-352.23180	0.00000	-352.23180	-300.84047
10	C	0.2917	50.26867	-352.63481	0.00000	-352.63481	-302.36614
11	C	0.2917	50.47500	-352.63481	0.00000	-352.63481	-302.15981
12	C	0.2913	52.10467	-352.23180	0.00000	-352.23180	-300.12713
13	C	0.8393	24.52133	-1014.78223	-0.00000	-1014.78223	-990.26090
14	C	0.8370	24.82167	-1011.96115	-0.00000	-1011.96115	-987.13949
15	C	0.8367	26.18800	-1011.55814	-0.00000	-1011.55814	-985.37014
16	C	0.8393	26.24867	-1014.78223	-0.00000	-1014.78223	-988.53357
17	C	-0.1770	31.53567	213.99895	-0.00000	213.99895	245.53462
18	C	-0.1773	30.83667	214.40196	-0.00000	214.40196	245.23863
19	C	-0.1773	29.06967	214.40196	-0.00000	214.40196	243.47163
20	C	-0.1770	28.89500	213.99895	-0.00000	213.99895	242.89395
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2080	38.02433	-251.47900	0.00000	-251.47900	-213.45466

24	C	0.2073	37.13433	-250.67297	-0.00000	-250.67297	-213.53864
25	C	1.0147	41.11600	-1226.76613	0.00000	-1226.76613	-1185.65013
26	C	1.0130	41.25800	-1224.75107	0.00000	-1224.75107	-1183.49307
27	C	1.0130	42.47933	-1224.75107	0.00000	-1224.75107	-1182.27174
28	C	1.0147	41.60900	-1226.76613	0.00000	-1226.76613	-1185.15713
29	C	0.2003	38.80000	-242.20974	0.00000	-242.20974	-203.40974
30	C	0.2003	39.43233	-242.20974	0.00000	-242.20974	-202.77741
31	C	0.2003	37.15733	-242.20974	0.00000	-242.20974	-205.05241
32	C	0.2003	38.04833	-242.20974	0.00000	-242.20974	-204.16141
33	C	0.0063	49.64767	-7.65721	-0.00000	-7.65721	41.99045
34	C	0.0067	49.67733	-8.06022	-0.00000	-8.06022	41.61711
35	C	0.0067	49.99767	-8.06022	-0.00000	-8.06022	41.93744
36	C	0.0063	51.50200	-7.65721	-0.00000	-7.65721	43.84479
A Average		0.8442	25.43796	-1020.62589	-0.00000	-1020.62589	-995.18794
B Average		1.0265	42.41408	-1241.07303	0.00000	-1241.07303	-1198.65894
M Average		0.2915	51.05992	-352.43331	0.00000	-352.43331	-301.37339

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FeL5-planar-HS-STO-PBE0-No-PSOSO
Temperature: 303
Spin: 2.5

atensor 1 C
0.755 0.070 0.015
0.070 1.541 0.154
0.015 0.154 0.831
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 2 C
0.754 -0.071 0.016
-0.071 1.540 -0.154
0.016 -0.154 0.830
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
0.754 -0.071 -0.016
-0.071 1.540 0.154
-0.016 0.154 0.830
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 C
0.755 0.070 -0.015
0.070 1.541 -0.154
-0.015 -0.154 0.831
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.746 0.807 0.148
0.807 1.849 0.397
0.148 0.397 -0.041
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 C
0.742 -0.808 0.144
-0.808 1.846 -0.394
0.144 -0.394 -0.047

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
0.743 -0.808 -0.144
-0.808 1.846 0.394
-0.144 0.394 -0.047
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 C
0.746 0.807 -0.148
0.807 1.849 -0.397
-0.148 -0.397 -0.041
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.210 0.590 0.152
0.590 0.210 0.119
0.152 0.119 0.457
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 C
0.211 -0.591 0.153
-0.591 0.210 -0.119
0.153 -0.119 0.457
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.211 -0.591 -0.153
-0.591 0.210 0.119
-0.153 0.119 0.457
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 C
0.210 0.590 -0.152
0.590 0.210 -0.119
-0.152 -0.119 0.457
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
1.880 0.825 0.244
0.825 0.723 0.098
0.244 0.098 -0.087
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 C
1.881 -0.825 0.240
-0.825 0.719 -0.094
0.240 -0.094 -0.091
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
1.880 -0.825 -0.240
-0.825 0.719 0.094
-0.240 0.094 -0.091
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 C
1.880 0.825 -0.244
0.825 0.723 -0.098
-0.244 -0.098 -0.087
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
-0.106 0.239 0.060
0.239 -0.103 0.029
0.060 0.029 -0.323
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 C
-0.106 -0.239 0.059
-0.239 -0.103 -0.028
0.059 -0.028 -0.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.106 -0.239 -0.059
-0.239 -0.103 0.028
-0.059 0.028 -0.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 C
-0.106 0.239 -0.060
0.239 -0.103 -0.029
-0.060 -0.029 -0.323
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 C
0.216 -0.135 0.019
-0.135 0.318 -0.011
0.019 -0.011 0.089
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 C
0.216 0.135 0.018
0.135 0.317 0.009
0.018 0.009 0.088
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 C
1.562 0.078 0.038

0.078 0.727 0.023
0.038 0.023 0.763
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 C
1.561 -0.077 0.038
-0.077 0.725 -0.023
0.038 -0.023 0.761
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 C
1.561 -0.077 -0.038
-0.077 0.725 0.023
-0.038 0.023 0.761
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 C
1.562 0.078 -0.038
0.078 0.727 -0.023
-0.038 -0.023 0.763
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 29 C
0.290 0.111 0.061
0.111 0.197 0.059
0.061 0.059 0.114
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 C
0.290 -0.111 0.060
-0.111 0.197 -0.058
0.060 -0.058 0.114
0.000 -0.001 0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 31 C
0.290 -0.111 -0.060
-0.111 0.197 0.058
-0.060 0.058 0.114
0.000 -0.001 -0.001
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 32 C
0.290 0.111 -0.061
0.111 0.197 -0.059
-0.061 -0.059 0.114
0.000 0.001 -0.001
0.001 0.000 0.000
0.000 0.000 0.000

atensor 33 C
0.020 0.092 0.003
0.092 0.046 -0.011
0.003 -0.011 -0.047
0.000 0.001 0.000

0.001 0.000 0.000
0.000 0.000 0.000

atensor 34 C
0.021 -0.092 0.002
-0.092 0.046 0.011
0.002 0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 35 C
0.021 -0.092 -0.002
-0.092 0.046 -0.011
-0.002 -0.011 -0.047
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 36 C
0.020 0.092 -0.003
0.092 0.046 0.011
-0.003 0.011 -0.047
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 37 C
0.035 0.082 0.037
0.082 0.015 0.020
0.037 0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 C
0.035 -0.082 0.037
-0.082 0.015 -0.019
0.037 -0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 39 C
0.035 -0.082 -0.037
-0.082 0.015 0.019
-0.037 0.019 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 40 C
0.035 0.082 -0.037
0.082 0.015 -0.020
-0.037 -0.020 -0.036
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 41 C
0.041 0.046 -0.003
0.046 0.039 0.021
-0.003 0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 42 C
0.041 -0.046 -0.003
-0.046 0.039 -0.021
-0.003 -0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 43 C
0.041 -0.046 0.003
-0.046 0.039 0.021
0.003 0.021 -0.029
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 44 C
0.041 0.046 0.003
0.046 0.039 -0.021
0.003 -0.021 -0.028
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 47 H
-0.116 0.407 0.085
0.407 1.135 0.297
0.085 0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 0.002
0.000 0.001 -0.001

atensor 48 H
-0.116 -0.408 0.084
-0.408 1.135 -0.295
0.084 -0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 49 H
-0.116 -0.408 -0.084
-0.408 1.135 0.295
-0.084 0.295 -0.239
-0.004 -0.001 0.000
-0.002 0.005 0.002
0.000 0.001 -0.001

atensor 50 H
-0.116 0.407 -0.085
0.407 1.135 -0.297
-0.085 -0.297 -0.237
-0.004 0.001 0.000
0.002 0.005 -0.002
0.000 -0.001 -0.001

atensor 51 H
-0.073 0.628 -0.167
0.628 0.430 -0.263
-0.167 -0.263 -0.421
0.000 0.005 -0.001
0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 52 H
-0.073 -0.629 -0.170
-0.629 0.429 0.268

-0.170 0.268 -0.419
0.000 -0.005 -0.001
-0.005 0.003 0.001
0.000 0.000 -0.001

atensor 53 H
-0.073 -0.629 0.170
-0.629 0.429 -0.268
0.170 -0.268 -0.419
0.000 -0.005 0.001
-0.005 0.003 -0.001
0.000 0.000 -0.001

atensor 54 H
-0.073 0.628 0.167
0.628 0.430 0.263
0.167 0.263 -0.421
0.000 0.005 0.001
0.005 0.003 0.001
0.000 0.000 -0.001

atensor 55 H
0.233 0.441 0.429
0.441 -0.126 0.276
0.429 0.276 -0.172
0.001 0.002 0.003
0.003 -0.001 0.002
0.001 0.001 0.000

atensor 56 H
0.234 -0.443 0.427
-0.443 -0.124 -0.275
0.427 -0.275 -0.175
0.001 -0.002 0.003
-0.003 -0.001 -0.002
0.001 -0.001 0.000

atensor 57 H
0.234 -0.443 -0.427
-0.443 -0.124 0.275
-0.427 0.275 -0.175
0.001 -0.002 -0.003
-0.003 -0.001 0.002
-0.001 0.001 0.000

atensor 58 H
0.233 0.441 -0.429
0.441 -0.126 -0.276
-0.429 -0.276 -0.172
0.001 0.002 -0.003
0.003 -0.001 -0.002
-0.001 -0.001 0.000

atensor 59 H
0.030 0.235 -0.038
0.235 0.155 -0.051
-0.038 -0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 60 H
0.030 -0.235 -0.039
-0.235 0.155 0.053
-0.039 0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000

0.000 0.000 0.000

atensor 61 H
0.030 -0.235 0.039
-0.235 0.155 -0.053
0.039 -0.053 -0.139
0.000 -0.002 0.000
-0.002 0.001 0.000
0.000 0.000 0.000

atensor 62 H
0.030 0.235 0.038
0.235 0.155 0.051
0.038 0.051 -0.140
0.000 0.002 0.000
0.002 0.001 0.000
0.000 0.000 0.000

atensor 63 H
1.208 0.430 0.099
0.430 -0.136 0.031
0.099 0.031 -0.311
0.005 0.002 0.002
0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 64 H
1.208 -0.429 0.096
-0.429 -0.137 -0.030
0.096 -0.030 -0.312
0.005 -0.002 0.002
-0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 65 H
1.208 -0.429 -0.096
-0.429 -0.137 0.030
-0.096 0.030 -0.312
0.005 -0.002 -0.002
-0.001 -0.004 0.001
0.000 0.000 -0.001

atensor 66 H
1.208 0.430 -0.099
0.430 -0.136 -0.031
-0.099 -0.031 -0.311
0.005 0.002 -0.002
0.001 -0.004 -0.001
0.000 0.000 -0.001

atensor 67 H
0.114 0.195 0.116
0.195 0.012 0.088
0.116 0.088 -0.085
0.001 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 68 H
0.114 -0.196 0.115
-0.196 0.013 -0.088
0.115 -0.088 -0.086
0.001 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 69 H

0.114 -0.196 -0.115
-0.196 0.013 0.088
-0.115 0.088 -0.086
0.001 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 70 H
0.114 0.195 -0.116
0.195 0.012 -0.088
-0.116 -0.088 -0.085
0.001 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 71 H
0.042 0.170 0.023
0.170 0.044 0.028
0.023 0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

atensor 72 H
0.042 -0.170 0.022
-0.170 0.044 -0.027
0.022 -0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 73 H
0.042 -0.170 -0.022
-0.170 0.044 0.027
-0.022 0.027 -0.130
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 74 H
0.042 0.170 -0.023
0.170 0.044 -0.028
-0.023 -0.028 -0.130
0.000 0.001 0.000
0.001 0.000 0.000
0.000 0.000 0.000

orbtensor 1 C
-222.856 -15.441 -1.797
-15.441 -302.054 -41.543
-1.797 -41.543 -87.648
261.510 -4.054 -0.922
-4.054 258.053 5.920
-0.922 5.920 222.696

orbtensor 2 C
-223.014 16.761 2.778
16.761 -299.984 41.884
2.778 41.884 -88.196
261.493 4.030 -1.127
4.030 258.060 -5.929
-1.127 -5.929 222.705

orbtensor 3 C
-223.132 16.202 -1.526
16.202 -300.516 -39.721
-1.526 -39.721 -89.594

261.493	4.030	1.125
4.030	258.060	5.931
1.125	5.931	222.706

orbtensor 4 C

-222.803	-16.997	0.252
-16.997	-301.519	44.429
0.252	44.429	-89.167
261.510	-4.053	0.920
-4.053	258.053	-5.918
0.920	-5.918	222.695

orbtensor 5 C

-283.518	-6.839	-2.496
-6.839	-297.188	-32.053
-2.496	-32.053	-109.849
270.694	2.204	0.455
2.204	265.836	4.951
0.455	4.951	228.872

orbtensor 6 C

-283.169	6.751	0.022
6.751	-293.464	34.072
0.022	34.072	-108.487
270.708	-2.227	0.285
-2.227	265.850	-4.902
0.285	-4.902	228.878

orbtensor 7 C

-281.417	5.524	2.548
5.524	-296.065	-33.489
2.548	-33.489	-111.853
270.706	-2.226	-0.286
-2.226	265.848	4.905
-0.286	4.905	228.877

orbtensor 8 C

-281.753	-6.301	0.116
-6.301	-296.147	33.055
0.116	33.055	-113.589
270.695	2.204	-0.457
2.204	265.836	-4.950
-0.457	-4.950	228.871

orbtensor 9 C

-256.114	-12.899	4.949
-12.899	-256.778	-21.424
4.949	-21.424	-75.935
262.817	0.522	0.776
0.522	262.852	2.900
0.776	2.900	217.332

orbtensor 10 C

-257.018	10.847	3.512
10.847	-258.260	20.675
3.512	20.675	-76.929
262.813	-0.536	0.627
-0.536	262.882	-2.748
0.627	-2.748	217.318

orbtensor 11 C

-258.134	12.197	-6.781
12.197	-257.286	-21.930
-6.781	-21.930	-76.167
262.814	-0.536	-0.628
-0.536	262.880	2.750
-0.628	2.750	217.318

orbtensor 12 C
-256.347 -11.281 -1.707
-11.281 -256.573 21.351
-1.707 21.351 -73.763
262.815 0.523 -0.778
0.523 262.852 -2.897
-0.778 -2.897 217.330

orbtensor 13 C
-298.065 -6.412 12.362
-6.412 -286.327 -3.750
12.362 -3.750 -107.790
266.304 2.067 -0.214
2.067 270.874 1.957
-0.214 1.957 228.568

orbtensor 14 C
-298.237 7.973 13.123
7.973 -284.550 3.905
13.123 3.905 -108.512
266.311 -2.065 -0.257
-2.065 270.892 -1.778
-0.257 -1.778 228.561

orbtensor 15 C
-299.216 7.653 -14.399
7.653 -283.915 -8.652
-14.399 -8.652 -104.072
266.312 -2.066 0.257
-2.066 270.892 1.781
0.257 1.781 228.563

orbtensor 16 C
-298.254 -5.534 -14.430
-5.534 -284.064 5.084
-14.430 5.084 -104.682
266.304 2.067 0.214
2.067 270.874 -1.954
0.214 -1.954 228.568

orbtensor 17 C
-217.551 -106.228 -56.647
-106.228 -227.046 47.957
-56.647 47.957 -217.887
252.329 14.873 10.149
14.873 254.103 -8.807
10.149 -8.807 250.659

orbtensor 18 C
-217.075 106.962 -55.380
106.962 -226.613 -48.087
-55.380 -48.087 -220.922
252.369 -14.901 10.063
-14.901 254.033 8.845
10.063 8.845 250.718

orbtensor 19 C
-220.287 107.565 57.620
107.565 -228.946 46.452
57.620 46.452 -220.680
252.374 -14.897 -10.067
-14.897 254.036 -8.849
-10.067 -8.849 250.712

orbtensor 20 C
-220.317 -108.397 55.496

-108.397 -228.227 -47.598
55.496 -47.598 -221.872
252.332 14.869 -10.151
14.869 254.109 8.809
-10.151 8.809 250.660

orbtensor 23 C
-189.408 69.892 85.922
69.892 -172.383 44.923
85.922 44.923 -269.970
245.741 -15.658 -6.123
-15.658 250.597 -12.110
-6.123 -12.110 249.496

orbtensor 24 C
-190.533 -70.911 85.463
-70.911 -171.824 -45.361
85.463 -45.361 -272.059
245.730 15.657 -6.199
15.657 250.691 12.075
-6.199 12.075 249.398

orbtensor 25 C
-307.696 -16.097 21.744
-16.097 -225.894 7.542
21.744 7.542 -85.351
258.883 -4.015 -2.040
-4.015 261.443 1.187
-2.040 1.187 221.963

orbtensor 26 C
-309.811 13.676 22.442
13.676 -221.257 -4.335
22.442 -4.335 -87.456
258.886 4.025 -2.027
4.025 261.456 -0.975
-2.027 -0.975 221.956

orbtensor 27 C
-308.240 14.531 -23.321
14.531 -219.568 9.035
-23.321 9.035 -87.052
258.887 4.024 2.029
4.024 261.456 0.978
2.029 0.978 221.955

orbtensor 28 C
-307.800 -16.844 -22.045
-16.844 -222.937 -2.501
-22.045 -2.501 -86.726
258.884 -4.015 2.041
-4.015 261.443 -1.185
2.041 -1.185 221.963

orbtensor 29 C
-161.790 -72.828 -44.309
-72.828 -204.988 86.462
-44.309 86.462 -261.856
247.878 14.961 13.443
14.961 246.760 -5.417
13.443 -5.417 250.396

orbtensor 30 C
-159.192 72.554 -41.267
72.554 -203.215 -85.844
-41.267 -85.844 -264.319
247.919 -15.018 13.383

-15.018 246.721 5.423
13.383 5.423 250.383

orbtensor 31 C
-164.283 71.804 42.844
71.804 -205.446 85.400
42.844 85.400 -263.825
247.929 -15.014 -13.385
-15.014 246.720 -5.428
-13.385 -5.428 250.377

orbtensor 32 C
-163.529 -72.412 43.416
-72.412 -203.840 -85.222
43.416 -85.222 -263.521
247.878 14.959 -13.446
14.959 246.764 5.419
-13.446 5.419 250.393

orbtensor 33 C
-152.629 -75.853 -41.131
-75.853 -200.352 95.170
-41.131 95.170 -233.250
244.306 15.918 10.860
15.918 244.351 -8.477
10.860 -8.477 246.517

orbtensor 34 C
-153.337 75.921 -39.832
75.921 -202.195 -93.379
-39.832 -93.379 -230.594
244.322 -15.957 10.787
-15.957 244.283 8.491
10.787 8.491 246.553

orbtensor 35 C
-151.330 77.267 43.691
77.267 -199.994 92.263
43.691 92.263 -233.838
244.330 -15.954 -10.790
-15.954 244.281 -8.497
-10.790 -8.497 246.544

orbtensor 36 C
-147.408 -75.655 45.476
-75.655 -201.719 -96.994
45.476 -96.994 -231.543
244.307 15.916 -10.863
15.916 244.355 8.478
-10.863 8.478 246.514

orbtensor 37 C
-184.308 -71.579 -96.166
-71.579 -157.953 42.683
-96.166 42.683 -240.461
242.769 16.007 9.554
16.007 246.572 -9.530
9.554 -9.530 246.313

orbtensor 38 C
-186.432 73.930 -95.546
73.930 -159.485 -41.347
-95.546 -41.347 -240.707
242.793 -16.032 9.485
-16.032 246.507 9.554
9.485 9.554 246.371

orbtensor 39 C
-186.961 72.882 98.050
72.882 -158.399 42.150
98.050 42.150 -239.645
242.801 -16.029 -9.488
-16.029 246.506 -9.560
-9.488 -9.560 246.363

orbtensor 40 C
-184.878 -73.069 96.556
-73.069 -160.540 -42.683
96.556 -42.683 -242.074
242.768 16.005 -9.557
16.005 246.575 9.531
-9.557 9.531 246.308

orbtensor 41 C
-196.270 -117.986 -57.600
-117.986 -207.488 46.829
-57.600 46.829 -184.913
243.818 12.812 10.677
12.812 245.851 -10.137
10.677 -10.137 250.681

orbtensor 42 C
-198.333 116.389 -56.673
116.389 -210.886 -46.776
-56.673 -46.776 -186.504
243.841 -12.844 10.631
-12.844 245.768 10.131
10.631 10.131 250.739

orbtensor 43 C
-197.668 118.936 57.375
118.936 -209.971 46.789
57.375 46.789 -183.741
243.849 -12.840 -10.634
-12.840 245.768 -10.137
-10.634 -10.137 250.730

orbtensor 44 C
-196.601 -117.647 57.945
-117.647 -210.663 -49.000
57.945 -49.000 -186.292
243.819 12.809 -10.680
12.809 245.854 10.138
-10.680 10.138 250.677

orbtensor 47 H
-3.449 -8.025 -1.380
-8.025 -15.587 -2.691
-1.380 -2.691 -5.092
35.460 4.745 -0.172
4.745 35.627 3.116
-0.172 3.116 18.711

orbtensor 48 H
-3.524 7.932 -1.571
7.932 -15.613 2.737
-1.571 2.737 -5.125
35.457 -4.755 -0.250
-4.755 35.626 -3.080
-0.250 -3.080 18.706

orbtensor 49 H
-3.429 7.924 1.298
7.924 -15.825 -2.619

1.298	-2.619	-4.804
35.456	-4.755	0.250
-4.755	35.626	3.082
0.250	3.082	18.706

orbtensor 50 H

-3.503	-7.956	1.704
-7.956	-15.697	2.894
1.704	2.894	-4.810
35.461	4.745	0.172
4.745	35.626	-3.116
0.172	-3.116	18.710

orbtensor 51 H

-8.548	-0.972	-9.078
-0.972	-3.572	-2.160
-9.078	-2.160	-16.494
31.287	4.573	5.532
4.573	27.487	-3.735
5.532	-3.735	34.496

orbtensor 52 H

-8.621	0.873	-8.930
0.873	-3.668	2.365
-8.930	2.365	-16.561
31.290	-4.598	5.519
-4.598	27.460	3.703
5.519	3.703	34.511

orbtensor 53 H

-8.688	0.664	8.816
0.664	-3.694	-2.451
8.816	-2.451	-16.551
31.294	-4.597	-5.520
-4.597	27.460	-3.706
-5.520	-3.706	34.506

orbtensor 54 H

-8.531	-0.841	9.044
-0.841	-3.667	2.424
9.044	2.424	-16.472
31.289	4.573	-5.532
4.573	27.488	3.736
-5.532	3.736	34.494

orbtensor 55 H

-3.571	-1.099	3.338
-1.099	-10.012	9.700
3.338	9.700	-14.591
26.832	4.401	3.615
4.401	32.581	-5.335
3.615	-5.335	34.284

orbtensor 56 H

-3.805	0.956	3.345
0.956	-9.968	-9.542
3.345	-9.542	-14.710
26.848	-4.400	3.615
-4.400	32.532	5.337
3.615	5.337	34.319

orbtensor 57 H

-3.852	0.858	-3.540
0.858	-10.175	9.510
-3.540	9.510	-14.702
26.850	-4.399	-3.617
-4.399	32.534	-5.338

-3.617 -5.338 34.316

orbtensor 58 H

-3.831 -0.835 -3.573
-0.835 -10.250 -9.460
-3.573 -9.460 -14.699
26.831 4.400 -3.617
4.400 32.583 5.336
-3.617 5.336 34.282

orbtensor 59 H

-1.057 -2.824 0.588
-2.824 -9.100 8.643
0.588 8.643 -11.960
26.917 4.379 0.302
4.379 33.312 -8.820
0.302 -8.820 33.689

orbtensor 60 H

-0.857 2.975 0.456
2.975 -8.731 -8.767
0.456 -8.767 -11.832
26.910 -4.358 0.298
-4.358 33.229 8.826
0.298 8.826 33.777

orbtensor 61 H

-0.775 3.192 -0.532
3.192 -8.567 8.940
-0.532 8.940 -11.581
26.911 -4.357 -0.300
-4.357 33.231 -8.827
-0.300 -8.827 33.773

orbtensor 62 H

-0.990 -3.119 -0.459
-3.119 -8.881 -8.996
-0.459 -8.996 -11.616
26.917 4.377 -0.305
4.377 33.314 8.821
-0.305 8.821 33.688

orbtensor 63 H

-16.081 -8.188 2.183
-8.188 -3.698 1.306
2.183 1.306 -4.684
36.175 4.783 -1.278
4.783 35.253 1.178
-1.278 1.178 18.423

orbtensor 64 H

-16.053 8.003 2.149
8.003 -3.776 -1.246
2.149 -1.246 -4.342
36.183 -4.777 -1.311
-4.777 35.259 -1.090
-1.311 -1.090 18.413

orbtensor 65 H

-16.299 7.959 -2.397
7.959 -3.548 1.290
-2.397 1.290 -4.701
36.183 -4.778 1.311
-4.778 35.260 1.091
1.311 1.091 18.413

orbtensor 66 H

-16.283	-8.089	-2.184
-8.089	-3.545	-1.260
-2.184	-1.260	-4.684
36.176	4.783	1.279
4.783	35.254	-1.177
1.279	-1.177	18.423

orbtensor 67 H

-7.725	-2.072	-8.240
-2.072	-1.305	0.096
-8.240	0.096	-13.178
31.850	3.758	8.935
3.758	27.157	-0.498
8.935	-0.498	35.029

orbtensor 68 H

-7.593	2.221	-8.512
2.221	-1.044	-0.151
-8.512	-0.151	-12.801
31.884	-3.806	8.924
-3.806	27.156	0.460
8.924	0.460	34.997

orbtensor 69 H

-7.302	2.401	8.589
2.401	-1.051	0.265
8.589	0.265	-12.952
31.889	-3.805	-8.925
-3.805	27.155	-0.463
-8.925	-0.463	34.992

orbtensor 70 H

-7.644	-2.124	8.411
-2.124	-1.117	-0.086
8.411	-0.086	-13.068
31.851	3.758	-8.936
3.758	27.157	0.499
-8.936	0.499	35.026

orbtensor 71 H

-8.801	-10.741	-1.794
-10.741	-9.317	0.495
-1.794	0.495	-2.211
33.480	9.739	2.342
9.739	34.042	-1.082
2.342	-1.082	26.828

orbtensor 72 H

-8.552	11.133	-2.028
11.133	-9.005	-0.865
-2.028	-0.865	-1.718
33.473	-9.749	2.278
-9.749	34.048	1.137
2.278	1.137	26.830

orbtensor 73 H

-8.356	11.370	2.206
11.370	-8.787	0.936
2.206	0.936	-1.875
33.477	-9.748	-2.278
-9.748	34.046	-1.139
-2.278	-1.139	26.828

orbtensor 74 H

-8.588	-11.065	1.969
-11.065	-9.008	-0.744
1.969	-0.744	-1.754

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33.479    9.738    -2.342
9.738    34.044    1.083
-2.342    1.083    26.827

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gtensor (ppt)
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000

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averaging
A Average:5,6,7,8,13,14,15,16
B Average:1,2,3,4,25,26,27,28
M Average:9,10,11,12

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	1.0423	43.23367	-1260.21606	0.00000	-1260.21606	-1216.98239
2	C	1.0413	43.68800	-1259.00703	0.00000	-1259.00703	-1215.31903
3	C	1.0413	43.00567	-1259.00703	0.00000	-1259.00703	-1216.00136
4	C	1.0423	42.92300	-1260.21606	0.00000	-1260.21606	-1217.29306
5	C	0.8513	24.94900	-1029.29064	-0.00000	-1029.29064	-1004.34164
6	C	0.8470	26.77200	-1024.05149	-0.00000	-1024.05149	-997.27949
7	C	0.8473	25.36533	-1024.45450	-0.00000	-1024.45450	-999.08917
8	C	0.8513	24.63767	-1029.29064	-0.00000	-1029.29064	-1004.65297
9	C	0.2923	51.39133	-353.44083	0.00000	-353.44083	-302.04950
10	C	0.2927	50.26867	-353.84384	0.00000	-353.84384	-303.57518
11	C	0.2927	50.47500	-353.84384	0.00000	-353.84384	-303.36884
12	C	0.2923	52.10467	-353.44083	0.00000	-353.44083	-301.33617
13	C	0.8387	24.52133	-1013.97621	-0.00000	-1013.97621	-989.45488
14	C	0.8363	24.82167	-1011.15513	-0.00000	-1011.15513	-986.33346
15	C	0.8360	26.18800	-1010.75212	-0.00000	-1010.75212	-984.56412
16	C	0.8387	26.24867	-1013.97621	-0.00000	-1013.97621	-987.72754
17	C	-0.1773	31.53567	214.40196	-0.00000	214.40196	245.93763
18	C	-0.1777	30.83667	214.80498	-0.00000	214.80498	245.64164
19	C	-0.1777	29.06967	214.80498	-0.00000	214.80498	243.87464
20	C	-0.1773	28.89500	214.40196	-0.00000	214.40196	243.29696
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2077	38.02433	-251.07599	-0.00000	-251.07599	-213.05165
24	C	0.2070	37.13433	-250.26996	-0.00000	-250.26996	-213.13563
25	C	1.0173	41.11600	-1229.99022	0.00000	-1229.99022	-1188.87422
26	C	1.0157	41.25800	-1227.97516	0.00000	-1227.97516	-1186.71716
27	C	1.0157	42.47933	-1227.97516	0.00000	-1227.97516	-1185.49583
28	C	1.0173	41.60900	-1229.99022	0.00000	-1229.99022	-1188.38122
29	C	0.2003	38.80000	-242.20974	0.00000	-242.20974	-203.40974
30	C	0.2003	39.43233	-242.20974	0.00000	-242.20974	-202.77741
31	C	0.2003	37.15733	-242.20974	0.00000	-242.20974	-205.05241
32	C	0.2003	38.04833	-242.20974	0.00000	-242.20974	-204.16141
33	C	0.0063	49.64767	-7.65721	-0.00000	-7.65721	41.99045
34	C	0.0067	49.67733	-8.06022	-0.00000	-8.06022	41.61711
35	C	0.0067	49.99767	-8.06022	-0.00000	-8.06022	41.93744
36	C	0.0063	51.50200	-7.65721	-0.00000	-7.65721	43.84479
A Average		0.8433	25.43796	-1019.61837	-0.00000	-1019.61837	-994.18041
B Average		1.0292	42.41408	-1244.29712	0.00000	-1244.29712	-1201.88303
M Average		0.2925	51.05992	-353.64234	0.00000	-353.64234	-302.58242

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FeL5-planar-HS-STO-PBE0-No-ZORA
Temperature: 303
Spin: 2.5

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Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	C	1.0490	43.23367	-1268.27628	0.00000	-1268.27628	-1225.04262
2	C	1.0487	43.68800	-1267.87327	0.00000	-1267.87327	-1224.18527
3	C	1.0487	43.00567	-1267.87327	0.00000	-1267.87327	-1224.86761
4	C	1.0490	42.92300	-1268.27628	0.00000	-1268.27628	-1225.35328
5	C	0.8150	24.94900	-985.36241	-0.00000	-985.36241	-960.41341
6	C	0.8107	26.77200	-980.12327	-0.00000	-980.12327	-953.35127
7	C	0.8107	25.36533	-980.12327	-0.00000	-980.12327	-954.75793
8	C	0.8147	24.63767	-984.95940	-0.00000	-984.95940	-960.32174
9	C	0.3180	51.39133	-384.47270	-0.00000	-384.47270	-333.08136
10	C	0.3183	50.26867	-384.87571	0.00000	-384.87571	-334.60704
11	C	0.3183	50.47500	-384.87571	0.00000	-384.87571	-334.40071
12	C	0.3177	52.10467	-384.06969	0.00000	-384.06969	-331.96502
13	C	0.8003	24.52133	-967.62992	-0.00000	-967.62992	-943.10859
14	C	0.7983	24.82167	-965.21185	0.00000	-965.21185	-940.39019
15	C	0.7983	26.18800	-965.21185	0.00000	-965.21185	-939.02385
16	C	0.8003	26.24867	-967.62992	-0.00000	-967.62992	-941.38125
17	C	-0.1887	31.53567	228.10435	0.00000	228.10435	259.64001
18	C	-0.1890	30.83667	228.50736	-0.00000	228.50736	259.34402
19	C	-0.1893	29.06967	228.91037	0.00000	228.91037	257.98004
20	C	-0.1887	28.89500	228.10435	0.00000	228.10435	256.99935
21	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	C	0.2197	38.02433	-265.58439	0.00000	-265.58439	-227.56006
24	C	0.2187	37.13433	-264.37536	0.00000	-264.37536	-227.24102
25	C	1.0233	41.11600	-1237.24442	-0.00000	-1237.24442	-1196.12842
26	C	1.0213	41.25800	-1234.82635	-0.00000	-1234.82635	-1193.56835
27	C	1.0213	42.47933	-1234.82635	-0.00000	-1234.82635	-1192.34702
28	C	1.0233	41.60900	-1237.24442	-0.00000	-1237.24442	-1195.63542
29	C	0.2113	38.80000	-255.50911	0.00000	-255.50911	-216.70911
30	C	0.2120	39.43233	-256.31513	-0.00000	-256.31513	-216.88280
31	C	0.2120	37.15733	-256.31513	-0.00000	-256.31513	-219.15780
32	C	0.2113	38.04833	-255.50911	0.00000	-255.50911	-217.46078
33	C	0.0063	49.64767	-7.65721	-0.00000	-7.65721	41.99045
34	C	0.0070	49.67733	-8.46324	-0.00000	-8.46324	41.21410
35	C	0.0070	49.99767	-8.46324	-0.00000	-8.46324	41.53443
36	C	0.0063	51.50200	-7.65721	-0.00000	-7.65721	43.84479
A Average		0.8060	25.43796	-974.53149	-0.00000	-974.53149	-949.09353
B Average		1.0356	42.41408	-1252.05508	-0.00000	-1252.05508	-1209.64100
M Average		0.3181	51.05992	-384.57345	0.00000	-384.57345	-333.51353

FeL3-STO-PBE0-Full
 Temperature: 298
 Spin: 2

atensor 2 H
 -0.192 -0.112 0.010
 -0.112 1.678 -0.370
 0.010 -0.370 -0.116
 -0.014 -0.005 0.000
 0.000 0.030 -0.006
 0.001 -0.010 -0.003

atensor 3 H
 -0.842 0.160 -0.103
 0.160 0.963 -1.094
 -0.103 -1.094 -0.128
 -0.019 0.001 0.001
 0.007 0.026 -0.024
 -0.001 -0.016 0.006

atensor 4 H
-0.681 -0.323 -0.105
-0.323 2.648 0.997
-0.105 0.997 -0.310
-0.025 -0.021 -0.005
-0.001 0.043 0.028
0.003 0.001 -0.015

atensor 5 H
-1.341 0.179 -0.532
0.179 -1.037 -1.338
-0.532 -1.338 2.768
-0.040 0.013 -0.016
0.013 -0.019 -0.043
-0.002 -0.009 0.039

atensor 6 H
-1.301 -0.224 -0.855
-0.224 -1.108 1.161
-0.855 1.161 2.750
-0.033 -0.002 -0.036
0.004 -0.034 0.020
-0.004 0.020 0.024

atensor 7 H
-0.769 0.515 -0.521
0.515 0.825 -1.845
-0.521 -1.845 0.875
-0.031 0.017 -0.009
0.017 0.017 -0.037
-0.004 -0.023 0.016

atensor 8 H
-1.567 -2.226 1.086
-2.226 3.204 -2.642
1.086 -2.642 -1.230
-0.038 -0.075 0.046
-0.046 0.086 -0.056
0.027 -0.037 -0.004

atensor 9 H
-0.057 0.664 0.811
0.664 1.099 1.694
0.810 1.694 1.423
-0.030 0.010 0.007
0.017 -0.006 0.031
0.007 0.013 -0.003

atensor 10 H
-0.963 0.052 1.447
0.052 -1.452 0.249
1.447 0.249 2.699
-0.032 0.012 0.035
0.000 -0.037 -0.015
0.019 0.009 0.022

atensor 11 H
-0.739 2.450 -0.454
2.450 2.415 -0.844
-0.454 -0.844 -1.886
-0.028 0.058 -0.004
0.059 0.048 -0.008
-0.019 -0.027 -0.015

atensor 12 H
0.353 -0.808 1.073

-0.808 0.881 -1.537
1.073 -1.537 1.631
-0.015 -0.020 0.036
-0.019 0.008 -0.038
0.018 -0.013 0.012

atensor 13 H
-0.546 -2.553 -0.495
-2.553 2.027 0.847
-0.495 0.847 -1.907
0.001 -0.075 -0.014
-0.053 0.055 0.031
0.006 0.005 -0.024

atensor 14 H
0.167 3.206 1.668
3.206 1.591 2.162
1.668 2.162 -1.328
-0.028 0.069 0.037
0.069 0.005 0.049
0.003 0.011 -0.030

atensor 15 H
-0.090 -0.930 -1.304
-0.930 0.058 1.379
-1.304 1.379 0.856
-0.002 -0.025 -0.037
-0.015 -0.008 0.033
-0.008 0.019 0.003

atensor 16 H
1.481 0.161 -1.864
0.161 -0.169 -0.149
-1.864 -0.149 1.699
0.015 0.009 -0.045
0.012 -0.027 -0.003
-0.023 0.005 0.015

atensor 17 H
0.940 0.450 1.827
0.450 -0.744 0.485
1.827 0.485 0.883
0.009 0.018 0.043
-0.003 -0.029 -0.004
0.015 0.008 -0.001

atensor 18 H
3.929 -0.981 -2.841
-0.981 -2.201 0.398
-2.840 0.398 -1.112
0.104 -0.016 -0.072
-0.018 -0.058 0.029
-0.036 0.022 -0.012

atensor 19 H
1.311 1.602 -0.822
1.602 0.262 -0.622
-0.822 -0.622 -0.481
0.021 0.040 -0.019
0.035 -0.002 -0.005
-0.022 -0.010 -0.004

atensor 20 H
0.311 -0.883 -0.918
-0.883 -0.289 0.682
-0.918 0.682 -0.119
0.016 -0.022 -0.027

-0.016 -0.003 0.019
-0.005 0.009 -0.002

atensor 21 H
3.438 0.180 0.949
0.180 -2.118 0.033
0.949 0.033 -1.916
0.093 0.014 0.029
-0.021 -0.042 0.004
0.001 0.011 -0.019

atensor 22 H
1.520 -1.268 0.932
-1.268 -0.718 -0.397
0.932 -0.397 -0.872
0.045 -0.028 0.029
-0.036 -0.004 -0.011
0.012 0.001 -0.008

atensor 23 H
0.617 0.652 1.010
0.652 -0.654 0.402
1.010 0.402 -0.172
0.015 0.018 0.024
0.006 -0.016 0.007
0.006 0.007 -0.008

atensor 24 H
1.049 0.901 0.265
0.901 0.315 0.177
0.265 0.177 -0.237
0.016 0.023 0.010
0.012 -0.007 0.006
-0.001 0.003 -0.008

atensor 25 H
1.332 -0.752 -0.328
-0.752 0.114 0.168
-0.328 0.168 -0.180
0.026 -0.017 -0.009
-0.021 -0.001 0.010
0.001 0.004 -0.006

orbtensor 2 H
2.618 3.772 2.100
3.772 -12.573 -3.389
2.100 -3.389 -0.691
19.493 -4.594 -2.859
-4.594 41.394 2.714
-2.859 2.714 24.860

orbtensor 3 H
2.765 0.436 3.987
0.436 -4.759 1.385
3.987 1.385 -8.208
19.739 0.009 -6.298
0.009 26.169 -3.951
-6.298 -3.951 38.517

orbtensor 4 H
4.331 -0.275 -0.315
-0.275 -6.695 -6.143
-0.315 -6.143 1.296
20.961 0.631 0.655
0.631 36.473 4.079
0.655 4.079 27.035

orbtensor 5 H
5.416 -0.672 1.484
-0.672 1.564 -0.448
1.484 -0.448 -5.348
24.542 -0.921 0.098
-0.921 25.493 1.913
0.098 1.913 34.100

orbtensor 6 H
2.684 0.522 -0.946
0.522 4.843 -0.888
-0.946 -0.888 -3.898
26.192 -0.001 1.734
-0.001 24.057 -1.078
1.734 -1.078 34.046

orbtensor 7 H
5.190 -3.141 0.721
-3.141 -3.344 3.315
0.721 3.315 0.710
24.840 3.394 0.038
3.394 32.616 -6.202
0.038 -6.202 24.987

orbtensor 8 H
4.984 5.752 -2.704
5.752 -7.178 2.611
-2.704 2.611 -2.454
25.658 -0.428 -2.501
-0.428 32.780 2.484
-2.501 2.484 27.933

orbtensor 9 H
5.914 -0.911 -0.731
-0.911 2.499 -4.861
-0.731 -4.861 -1.337
23.749 1.198 3.373
1.198 29.242 7.479
3.373 7.479 29.584

orbtensor 10 H
3.804 -1.506 -0.206
-1.506 4.149 2.225
-0.206 2.225 -3.781
24.519 0.850 -1.727
0.850 25.552 -0.787
-1.727 -0.787 34.139

orbtensor 11 H
2.172 -2.024 0.945
-2.024 -8.164 3.443
0.945 3.443 2.265
26.384 -2.146 2.341
-2.146 35.753 0.935
2.341 0.935 24.477

orbtensor 12 H
3.564 2.126 -4.832
2.126 2.310 3.752
-4.832 3.752 -3.071
26.695 -2.801 4.835
-2.801 25.914 -6.637
4.835 -6.637 30.006

orbtensor 13 H
-5.447 5.573 2.177
5.573 -2.940 -2.477

2.177	-2.477	3.099
35.155	-3.160	-0.838
-3.160	26.821	-2.376
-0.838	-2.376	24.595

orbtensor 14 H

3.673	-6.512	-0.759
-6.512	0.428	-1.453
-0.759	-1.453	0.069
30.649	3.107	-1.084
3.107	27.815	-3.437
-1.084	-3.437	27.911

orbtensor 15 H

0.950	4.303	2.432
4.303	1.030	-2.679
2.432	-2.679	2.002
27.493	-5.030	-5.394
-5.030	29.735	3.162
-5.394	3.162	25.254

orbtensor 16 H

1.275	-1.665	5.547
-1.665	5.274	1.380
5.547	1.380	-3.247
28.364	1.764	-8.146
1.764	23.957	-0.923
-8.146	-0.923	30.056

orbtensor 17 H

-2.649	-1.684	-3.056
-1.684	5.336	-0.397
-3.056	-0.397	2.313
33.601	1.753	5.321
1.753	23.951	3.155
5.321	3.155	25.064

orbtensor 18 H

-8.731	1.536	3.132
1.536	6.856	-2.078
3.132	-2.078	-1.619
31.330	-2.833	3.378
-2.833	27.087	0.964
3.378	0.964	27.901

orbtensor 19 H

-4.398	-5.014	6.189
-5.014	1.893	3.008
6.189	3.008	0.075
32.890	6.516	-3.854
6.516	24.415	-1.796
-3.854	-1.796	27.117

orbtensor 20 H

-3.797	2.432	-1.058
2.432	1.233	-4.714
-1.058	-4.714	-7.298
24.641	-2.404	0.084
-2.404	21.356	7.786
0.084	7.786	38.278

orbtensor 21 H

-8.317	-2.926	-2.950
-2.926	0.208	-1.942
-2.950	-1.942	2.550
31.700	5.259	-1.757
5.259	30.191	1.864

-1.757 1.864 24.588

orbtensor 22 H

-4.415 5.586 -5.877
5.586 0.082 2.996
-5.877 2.996 0.532
31.881 -7.026 3.306
-7.026 25.374 -2.597
3.306 -2.597 26.949

orbtensor 23 H

-2.127 -2.745 -3.396
-2.745 0.398 3.320
-3.396 3.320 -6.513
24.812 2.476 7.218
2.476 21.828 -4.046
7.218 -4.046 37.739

orbtensor 24 H

-4.701 -8.223 1.800
-8.223 -4.738 3.597
1.800 3.597 0.140
30.992 11.788 -0.412
11.788 30.038 -3.939
-0.412 -3.939 24.445

orbtensor 25 H

-13.016 4.356 -3.999
4.356 2.017 -0.721
-3.999 -0.721 0.035
40.593 -6.440 3.185
-6.440 20.451 1.540
3.185 1.540 24.366

gtensor (ppt)

-0.191 0.010 0.000
0.010 -0.183 -0.001
0.000 -0.001 -0.168
51.211 -9.120 -4.036
-9.120 43.699 -10.014
-4.036 -10.014 21.060

zfstensor (cm-1)

-1.660434 1.196072 0.127590
1.196072 -0.654720 0.323328
0.127590 0.323328 1.163305

averaging

Cis Average:3,20,23

Trans Average:2,24,25

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4610	25.03367	-99.61981	-1.26709	-100.88690	-75.85324
3	H	0.0020	24.74100	-0.43219	-0.34202	-0.77421	23.96679
4	H	0.5533	27.80033	-119.57259	-0.26424	-119.83682	-92.03649
5	H	0.1233	28.58900	-26.65172	5.82214	-20.82959	7.75941
6	H	0.0993	29.30800	-21.46544	7.54278	-13.92266	15.38534
7	H	0.3110	28.33300	-67.20556	1.20392	-66.00164	-37.66864
8	H	0.1503	27.24100	-32.48629	-9.29967	-41.78595	-14.54495
9	H	0.8087	29.88367	-174.74885	6.21375	-168.53510	-138.65144
10	H	0.0790	29.46067	-17.07151	7.78418	-9.28733	20.17334
11	H	-0.0683	27.62900	14.76649	1.66654	16.43303	44.06203
12	H	0.9567	28.47267	-206.73092	-1.23627	-207.96719	-179.49452

13	H	-0.1313	27.09433	28.38048	-8.93590	19.44458	46.53891
14	H	0.1257	30.18167	-27.15594	8.09426	-19.06169	11.11998
15	H	0.2723	28.82133	-58.84988	0.34046	-58.50942	-29.68809
16	H	1.0047	28.55967	-217.10348	0.37070	-216.73278	-188.17311
17	H	0.3527	29.20533	-76.20952	3.04897	-73.16055	-43.95521
18	H	0.2167	27.60800	-46.82059	-9.94374	-56.76433	-29.15633
19	H	0.3690	27.33067	-79.73907	0.05793	-79.68113	-52.35047
20	H	-0.0287	24.80433	6.19472	-2.35320	3.84153	28.64586
21	H	-0.1880	26.97333	40.62587	-6.53282	34.09305	61.06638
22	H	-0.0123	26.80100	2.66517	-6.59833	-3.93315	22.86785
23	H	-0.0727	25.37900	15.70291	1.61611	17.31902	42.69802
24	H	0.3760	25.39200	-81.25173	0.54524	-80.70649	-55.31449
25	H	0.4283	24.81533	-92.56071	-4.05063	-96.61133	-71.79600
Cis Average		-0.0331	24.97478	7.15515	-0.35970	6.79544	31.77022
Trans Average		0.4218	25.08033	-91.14408	-1.59083	-92.73491	-67.65458

=====

FeL3-STO-PBE0-No-ZFS

Temperature: 298

Spin: 2

atensor 2 H

-0.192 -0.112 0.010
-0.112 1.678 -0.370
0.010 -0.370 -0.116
-0.014 -0.005 0.000
0.000 0.030 -0.006
0.001 -0.010 -0.003

atensor 3 H

-0.842 0.160 -0.103
0.160 0.963 -1.094
-0.103 -1.094 -0.128
-0.019 0.001 0.001
0.007 0.026 -0.024
-0.001 -0.016 0.006

atensor 4 H

-0.681 -0.323 -0.105
-0.323 2.648 0.997
-0.105 0.997 -0.310
-0.025 -0.021 -0.005
-0.001 0.043 0.028
0.003 0.001 -0.015

atensor 5 H

-1.341 0.179 -0.532
0.179 -1.037 -1.338
-0.532 -1.338 2.768
-0.040 0.013 -0.016
0.013 -0.019 -0.043
-0.002 -0.009 0.039

atensor 6 H

-1.301 -0.224 -0.855
-0.224 -1.108 1.161
-0.855 1.161 2.750
-0.033 -0.002 -0.036
0.004 -0.034 0.020
-0.004 0.020 0.024

atensor 7 H

-0.769 0.515 -0.521
0.515 0.825 -1.845
-0.521 -1.845 0.875
-0.031 0.017 -0.009

0.017 0.017 -0.037
-0.004 -0.023 0.016

atensor 8 H
-1.567 -2.226 1.086
-2.226 3.204 -2.642
1.086 -2.642 -1.230
-0.038 -0.075 0.046
-0.046 0.086 -0.056
0.027 -0.037 -0.004

atensor 9 H
-0.057 0.664 0.811
0.664 1.099 1.694
0.810 1.694 1.423
-0.030 0.010 0.007
0.017 -0.006 0.031
0.007 0.013 -0.003

atensor 10 H
-0.963 0.052 1.447
0.052 -1.452 0.249
1.447 0.249 2.699
-0.032 0.012 0.035
0.000 -0.037 -0.015
0.019 0.009 0.022

atensor 11 H
-0.739 2.450 -0.454
2.450 2.415 -0.844
-0.454 -0.844 -1.886
-0.028 0.058 -0.004
0.059 0.048 -0.008
-0.019 -0.027 -0.015

atensor 12 H
0.353 -0.808 1.073
-0.808 0.881 -1.537
1.073 -1.537 1.631
-0.015 -0.020 0.036
-0.019 0.008 -0.038
0.018 -0.013 0.012

atensor 13 H
-0.546 -2.553 -0.495
-2.553 2.027 0.847
-0.495 0.847 -1.907
0.001 -0.075 -0.014
-0.053 0.055 0.031
0.006 0.005 -0.024

atensor 14 H
0.167 3.206 1.668
3.206 1.591 2.162
1.668 2.162 -1.328
-0.028 0.069 0.037
0.069 0.005 0.049
0.003 0.011 -0.030

atensor 15 H
-0.090 -0.930 -1.304
-0.930 0.058 1.379
-1.304 1.379 0.856
-0.002 -0.025 -0.037
-0.015 -0.008 0.033
-0.008 0.019 0.003

atensor 16 H
1.481 0.161 -1.864
0.161 -0.169 -0.149
-1.864 -0.149 1.699
0.015 0.009 -0.045
0.012 -0.027 -0.003
-0.023 0.005 0.015

atensor 17 H
0.940 0.450 1.827
0.450 -0.744 0.485
1.827 0.485 0.883
0.009 0.018 0.043
-0.003 -0.029 -0.004
0.015 0.008 -0.001

atensor 18 H
3.929 -0.981 -2.841
-0.981 -2.201 0.398
-2.840 0.398 -1.112
0.104 -0.016 -0.072
-0.018 -0.058 0.029
-0.036 0.022 -0.012

atensor 19 H
1.311 1.602 -0.822
1.602 0.262 -0.622
-0.822 -0.622 -0.481
0.021 0.040 -0.019
0.035 -0.002 -0.005
-0.022 -0.010 -0.004

atensor 20 H
0.311 -0.883 -0.918
-0.883 -0.289 0.682
-0.918 0.682 -0.119
0.016 -0.022 -0.027
-0.016 -0.003 0.019
-0.005 0.009 -0.002

atensor 21 H
3.438 0.180 0.949
0.180 -2.118 0.033
0.949 0.033 -1.916
0.093 0.014 0.029
-0.021 -0.042 0.004
0.001 0.011 -0.019

atensor 22 H
1.520 -1.268 0.932
-1.268 -0.718 -0.397
0.932 -0.397 -0.872
0.045 -0.028 0.029
-0.036 -0.004 -0.011
0.012 0.001 -0.008

atensor 23 H
0.617 0.652 1.010
0.652 -0.654 0.402
1.010 0.402 -0.172
0.015 0.018 0.024
0.006 -0.016 0.007
0.006 0.007 -0.008

atensor 24 H
1.049 0.901 0.265
0.901 0.315 0.177

0.265 0.177 -0.237
0.016 0.023 0.010
0.012 -0.007 0.006
-0.001 0.003 -0.008

atensor 25 H
1.332 -0.752 -0.328
-0.752 0.114 0.168
-0.328 0.168 -0.180
0.026 -0.017 -0.009
-0.021 -0.001 0.010
0.001 0.004 -0.006

orbtensor 2 H
2.618 3.772 2.100
3.772 -12.573 -3.389
2.100 -3.389 -0.691
19.493 -4.594 -2.859
-4.594 41.394 2.714
-2.859 2.714 24.860

orbtensor 3 H
2.765 0.436 3.987
0.436 -4.759 1.385
3.987 1.385 -8.208
19.739 0.009 -6.298
0.009 26.169 -3.951
-6.298 -3.951 38.517

orbtensor 4 H
4.331 -0.275 -0.315
-0.275 -6.695 -6.143
-0.315 -6.143 1.296
20.961 0.631 0.655
0.631 36.473 4.079
0.655 4.079 27.035

orbtensor 5 H
5.416 -0.672 1.484
-0.672 1.564 -0.448
1.484 -0.448 -5.348
24.542 -0.921 0.098
-0.921 25.493 1.913
0.098 1.913 34.100

orbtensor 6 H
2.684 0.522 -0.946
0.522 4.843 -0.888
-0.946 -0.888 -3.898
26.192 -0.001 1.734
-0.001 24.057 -1.078
1.734 -1.078 34.046

orbtensor 7 H
5.190 -3.141 0.721
-3.141 -3.344 3.315
0.721 3.315 0.710
24.840 3.394 0.038
3.394 32.616 -6.202
0.038 -6.202 24.987

orbtensor 8 H
4.984 5.752 -2.704
5.752 -7.178 2.611
-2.704 2.611 -2.454
25.658 -0.428 -2.501
-0.428 32.780 2.484

-2.501 2.484 27.933

orbtensor 9 H

5.914 -0.911 -0.731
-0.911 2.499 -4.861
-0.731 -4.861 -1.337
23.749 1.198 3.373
1.198 29.242 7.479
3.373 7.479 29.584

orbtensor 10 H

3.804 -1.506 -0.206
-1.506 4.149 2.225
-0.206 2.225 -3.781
24.519 0.850 -1.727
0.850 25.552 -0.787
-1.727 -0.787 34.139

orbtensor 11 H

2.172 -2.024 0.945
-2.024 -8.164 3.443
0.945 3.443 2.265
26.384 -2.146 2.341
-2.146 35.753 0.935
2.341 0.935 24.477

orbtensor 12 H

3.564 2.126 -4.832
2.126 2.310 3.752
-4.832 3.752 -3.071
26.695 -2.801 4.835
-2.801 25.914 -6.637
4.835 -6.637 30.006

orbtensor 13 H

-5.447 5.573 2.177
5.573 -2.940 -2.477
2.177 -2.477 3.099
35.155 -3.160 -0.838
-3.160 26.821 -2.376
-0.838 -2.376 24.595

orbtensor 14 H

3.673 -6.512 -0.759
-6.512 0.428 -1.453
-0.759 -1.453 0.069
30.649 3.107 -1.084
3.107 27.815 -3.437
-1.084 -3.437 27.911

orbtensor 15 H

0.950 4.303 2.432
4.303 1.030 -2.679
2.432 -2.679 2.002
27.493 -5.030 -5.394
-5.030 29.735 3.162
-5.394 3.162 25.254

orbtensor 16 H

1.275 -1.665 5.547
-1.665 5.274 1.380
5.547 1.380 -3.247
28.364 1.764 -8.146
1.764 23.957 -0.923
-8.146 -0.923 30.056

orbtensor 17 H

-2.649	-1.684	-3.056
-1.684	5.336	-0.397
-3.056	-0.397	2.313
33.601	1.753	5.321
1.753	23.951	3.155
5.321	3.155	25.064

orbtensor 18 H

-8.731	1.536	3.132
1.536	6.856	-2.078
3.132	-2.078	-1.619
31.330	-2.833	3.378
-2.833	27.087	0.964
3.378	0.964	27.901

orbtensor 19 H

-4.398	-5.014	6.189
-5.014	1.893	3.008
6.189	3.008	0.075
32.890	6.516	-3.854
6.516	24.415	-1.796
-3.854	-1.796	27.117

orbtensor 20 H

-3.797	2.432	-1.058
2.432	1.233	-4.714
-1.058	-4.714	-7.298
24.641	-2.404	0.084
-2.404	21.356	7.786
0.084	7.786	38.278

orbtensor 21 H

-8.317	-2.926	-2.950
-2.926	0.208	-1.942
-2.950	-1.942	2.550
31.700	5.259	-1.757
5.259	30.191	1.864
-1.757	1.864	24.588

orbtensor 22 H

-4.415	5.586	-5.877
5.586	0.082	2.996
-5.877	2.996	0.532
31.881	-7.026	3.306
-7.026	25.374	-2.597
3.306	-2.597	26.949

orbtensor 23 H

-2.127	-2.745	-3.396
-2.745	0.398	3.320
-3.396	3.320	-6.513
24.812	2.476	7.218
2.476	21.828	-4.046
7.218	-4.046	37.739

orbtensor 24 H

-4.701	-8.223	1.800
-8.223	-4.738	3.597
1.800	3.597	0.140
30.992	11.788	-0.412
11.788	30.038	-3.939
-0.412	-3.939	24.445

orbtensor 25 H

-13.016	4.356	-3.999
4.356	2.017	-0.721
-3.999	-0.721	0.035

```

40.593   -6.440   3.185
-6.440   20.451   1.540
3.185    1.540   24.366

```

```

gtensor (ppt)
-0.191   0.010   0.000
0.010   -0.183   -0.001
0.000   -0.001   -0.168
51.211  -9.120   -4.036
-9.120   43.699  -10.014
-4.036  -10.014  21.060

```

```

averaging
Cis Average:3,20,23
Trans Average:2,24,25

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4610	25.03367	-99.61347	-0.62433	-100.23780	-75.20413
3	H	0.0020	24.74100	-0.43216	-0.58186	-1.01402	23.72698
4	H	0.5533	27.80033	-119.56497	0.10228	-119.46270	-91.66236
5	H	0.1233	28.58900	-26.65002	1.54636	-25.10366	3.48534
6	H	0.0993	29.30800	-21.46407	2.95749	-18.50658	10.80142
7	H	0.3110	28.33300	-67.20128	-0.37631	-67.57759	-39.24459
8	H	0.1503	27.24100	-32.48422	-3.69161	-36.17583	-8.93483
9	H	0.8087	29.88367	-174.73772	2.60701	-172.13071	-142.24705
10	H	0.0790	29.46067	-17.07042	3.02516	-14.04526	15.41541
11	H	-0.0683	27.62900	14.76555	-0.40686	14.35869	41.98769
12	H	0.9567	28.47267	-206.71775	-0.61145	-207.32920	-178.85654
13	H	-0.1313	27.09433	28.37867	-2.54097	25.83770	52.93203
14	H	0.1257	30.18167	-27.15421	2.94826	-24.20595	5.97572
15	H	0.2723	28.82133	-58.84613	0.56937	-58.27676	-29.45543
16	H	1.0047	28.55967	-217.08965	-0.09880	-217.18845	-188.62879
17	H	0.3527	29.20533	-76.20466	1.43196	-74.77271	-45.56737
18	H	0.2167	27.60800	-46.81761	-3.24822	-50.06583	-22.45783
19	H	0.3690	27.33067	-79.73399	-0.56770	-80.30169	-52.97103
20	H	-0.0287	24.80433	6.19433	-0.52202	5.67231	30.47665
21	H	-0.1880	26.97333	40.62328	-1.96314	38.66014	65.63347
22	H	-0.0123	26.80100	2.66500	-1.95936	0.70564	27.50664
23	H	-0.0727	25.37900	15.70191	0.73580	16.43771	41.81671
24	H	0.3760	25.39200	-81.24656	0.11739	-81.12917	-55.73717
25	H	0.4283	24.81533	-92.55481	-1.20341	-93.75823	-68.94289
Cis Average		-0.0331	24.97478	7.15469	-0.12269	7.03200	32.00678
Trans Average		0.4218	25.08033	-91.13828	-0.57012	-91.70840	-66.62806

```

=====
FeL3-STO-PBE0-No-G
Temperature: 298
Spin: 2

```

```

atensor 2 H
-0.192 -0.112 0.010
-0.112 1.678 -0.370
0.010 -0.370 -0.116
-0.014 -0.005 0.000
0.000 0.030 -0.006
0.001 -0.010 -0.003

```

```

atensor 3 H
-0.842 0.160 -0.103
0.160 0.963 -1.094
-0.103 -1.094 -0.128
-0.019 0.001 0.001

```

0.007 0.026 -0.024
-0.001 -0.016 0.006

atensor 4 H
-0.681 -0.323 -0.105
-0.323 2.648 0.997
-0.105 0.997 -0.310
-0.025 -0.021 -0.005
-0.001 0.043 0.028
0.003 0.001 -0.015

atensor 5 H
-1.341 0.179 -0.532
0.179 -1.037 -1.338
-0.532 -1.338 2.768
-0.040 0.013 -0.016
0.013 -0.019 -0.043
-0.002 -0.009 0.039

atensor 6 H
-1.301 -0.224 -0.855
-0.224 -1.108 1.161
-0.855 1.161 2.750
-0.033 -0.002 -0.036
0.004 -0.034 0.020
-0.004 0.020 0.024

atensor 7 H
-0.769 0.515 -0.521
0.515 0.825 -1.845
-0.521 -1.845 0.875
-0.031 0.017 -0.009
0.017 0.017 -0.037
-0.004 -0.023 0.016

atensor 8 H
-1.567 -2.226 1.086
-2.226 3.204 -2.642
1.086 -2.642 -1.230
-0.038 -0.075 0.046
-0.046 0.086 -0.056
0.027 -0.037 -0.004

atensor 9 H
-0.057 0.664 0.811
0.664 1.099 1.694
0.810 1.694 1.423
-0.030 0.010 0.007
0.017 -0.006 0.031
0.007 0.013 -0.003

atensor 10 H
-0.963 0.052 1.447
0.052 -1.452 0.249
1.447 0.249 2.699
-0.032 0.012 0.035
0.000 -0.037 -0.015
0.019 0.009 0.022

atensor 11 H
-0.739 2.450 -0.454
2.450 2.415 -0.844
-0.454 -0.844 -1.886
-0.028 0.058 -0.004
0.059 0.048 -0.008
-0.019 -0.027 -0.015

atensor 12 H
0.353 -0.808 1.073
-0.808 0.881 -1.537
1.073 -1.537 1.631
-0.015 -0.020 0.036
-0.019 0.008 -0.038
0.018 -0.013 0.012

atensor 13 H
-0.546 -2.553 -0.495
-2.553 2.027 0.847
-0.495 0.847 -1.907
0.001 -0.075 -0.014
-0.053 0.055 0.031
0.006 0.005 -0.024

atensor 14 H
0.167 3.206 1.668
3.206 1.591 2.162
1.668 2.162 -1.328
-0.028 0.069 0.037
0.069 0.005 0.049
0.003 0.011 -0.030

atensor 15 H
-0.090 -0.930 -1.304
-0.930 0.058 1.379
-1.304 1.379 0.856
-0.002 -0.025 -0.037
-0.015 -0.008 0.033
-0.008 0.019 0.003

atensor 16 H
1.481 0.161 -1.864
0.161 -0.169 -0.149
-1.864 -0.149 1.699
0.015 0.009 -0.045
0.012 -0.027 -0.003
-0.023 0.005 0.015

atensor 17 H
0.940 0.450 1.827
0.450 -0.744 0.485
1.827 0.485 0.883
0.009 0.018 0.043
-0.003 -0.029 -0.004
0.015 0.008 -0.001

atensor 18 H
3.929 -0.981 -2.841
-0.981 -2.201 0.398
-2.840 0.398 -1.112
0.104 -0.016 -0.072
-0.018 -0.058 0.029
-0.036 0.022 -0.012

atensor 19 H
1.311 1.602 -0.822
1.602 0.262 -0.622
-0.822 -0.622 -0.481
0.021 0.040 -0.019
0.035 -0.002 -0.005
-0.022 -0.010 -0.004

atensor 20 H
0.311 -0.883 -0.918
-0.883 -0.289 0.682

-0.918 0.682 -0.119
0.016 -0.022 -0.027
-0.016 -0.003 0.019
-0.005 0.009 -0.002

atensor 21 H
3.438 0.180 0.949
0.180 -2.118 0.033
0.949 0.033 -1.916
0.093 0.014 0.029
-0.021 -0.042 0.004
0.001 0.011 -0.019

atensor 22 H
1.520 -1.268 0.932
-1.268 -0.718 -0.397
0.932 -0.397 -0.872
0.045 -0.028 0.029
-0.036 -0.004 -0.011
0.012 0.001 -0.008

atensor 23 H
0.617 0.652 1.010
0.652 -0.654 0.402
1.010 0.402 -0.172
0.015 0.018 0.024
0.006 -0.016 0.007
0.006 0.007 -0.008

atensor 24 H
1.049 0.901 0.265
0.901 0.315 0.177
0.265 0.177 -0.237
0.016 0.023 0.010
0.012 -0.007 0.006
-0.001 0.003 -0.008

atensor 25 H
1.332 -0.752 -0.328
-0.752 0.114 0.168
-0.328 0.168 -0.180
0.026 -0.017 -0.009
-0.021 -0.001 0.010
0.001 0.004 -0.006

orbtensor 2 H
2.618 3.772 2.100
3.772 -12.573 -3.389
2.100 -3.389 -0.691
19.493 -4.594 -2.859
-4.594 41.394 2.714
-2.859 2.714 24.860

orbtensor 3 H
2.765 0.436 3.987
0.436 -4.759 1.385
3.987 1.385 -8.208
19.739 0.009 -6.298
0.009 26.169 -3.951
-6.298 -3.951 38.517

orbtensor 4 H
4.331 -0.275 -0.315
-0.275 -6.695 -6.143
-0.315 -6.143 1.296
20.961 0.631 0.655
0.631 36.473 4.079

0.655 4.079 27.035

orbtensor 5 H

5.416 -0.672 1.484
-0.672 1.564 -0.448
1.484 -0.448 -5.348
24.542 -0.921 0.098
-0.921 25.493 1.913
0.098 1.913 34.100

orbtensor 6 H

2.684 0.522 -0.946
0.522 4.843 -0.888
-0.946 -0.888 -3.898
26.192 -0.001 1.734
-0.001 24.057 -1.078
1.734 -1.078 34.046

orbtensor 7 H

5.190 -3.141 0.721
-3.141 -3.344 3.315
0.721 3.315 0.710
24.840 3.394 0.038
3.394 32.616 -6.202
0.038 -6.202 24.987

orbtensor 8 H

4.984 5.752 -2.704
5.752 -7.178 2.611
-2.704 2.611 -2.454
25.658 -0.428 -2.501
-0.428 32.780 2.484
-2.501 2.484 27.933

orbtensor 9 H

5.914 -0.911 -0.731
-0.911 2.499 -4.861
-0.731 -4.861 -1.337
23.749 1.198 3.373
1.198 29.242 7.479
3.373 7.479 29.584

orbtensor 10 H

3.804 -1.506 -0.206
-1.506 4.149 2.225
-0.206 2.225 -3.781
24.519 0.850 -1.727
0.850 25.552 -0.787
-1.727 -0.787 34.139

orbtensor 11 H

2.172 -2.024 0.945
-2.024 -8.164 3.443
0.945 3.443 2.265
26.384 -2.146 2.341
-2.146 35.753 0.935
2.341 0.935 24.477

orbtensor 12 H

3.564 2.126 -4.832
2.126 2.310 3.752
-4.832 3.752 -3.071
26.695 -2.801 4.835
-2.801 25.914 -6.637
4.835 -6.637 30.006

orbtensor 13 H

-5.447	5.573	2.177
5.573	-2.940	-2.477
2.177	-2.477	3.099
35.155	-3.160	-0.838
-3.160	26.821	-2.376
-0.838	-2.376	24.595

orbtensor 14 H

3.673	-6.512	-0.759
-6.512	0.428	-1.453
-0.759	-1.453	0.069
30.649	3.107	-1.084
3.107	27.815	-3.437
-1.084	-3.437	27.911

orbtensor 15 H

0.950	4.303	2.432
4.303	1.030	-2.679
2.432	-2.679	2.002
27.493	-5.030	-5.394
-5.030	29.735	3.162
-5.394	3.162	25.254

orbtensor 16 H

1.275	-1.665	5.547
-1.665	5.274	1.380
5.547	1.380	-3.247
28.364	1.764	-8.146
1.764	23.957	-0.923
-8.146	-0.923	30.056

orbtensor 17 H

-2.649	-1.684	-3.056
-1.684	5.336	-0.397
-3.056	-0.397	2.313
33.601	1.753	5.321
1.753	23.951	3.155
5.321	3.155	25.064

orbtensor 18 H

-8.731	1.536	3.132
1.536	6.856	-2.078
3.132	-2.078	-1.619
31.330	-2.833	3.378
-2.833	27.087	0.964
3.378	0.964	27.901

orbtensor 19 H

-4.398	-5.014	6.189
-5.014	1.893	3.008
6.189	3.008	0.075
32.890	6.516	-3.854
6.516	24.415	-1.796
-3.854	-1.796	27.117

orbtensor 20 H

-3.797	2.432	-1.058
2.432	1.233	-4.714
-1.058	-4.714	-7.298
24.641	-2.404	0.084
-2.404	21.356	7.786
0.084	7.786	38.278

orbtensor 21 H

-8.317	-2.926	-2.950
-2.926	0.208	-1.942
-2.950	-1.942	2.550

```

31.700    5.259    -1.757
5.259    30.191    1.864
-1.757    1.864    24.588

```

```

orbtensor 22 H
-4.415    5.586    -5.877
5.586    0.082    2.996
-5.877    2.996    0.532
31.881    -7.026    3.306
-7.026    25.374    -2.597
3.306    -2.597    26.949

```

```

orbtensor 23 H
-2.127    -2.745    -3.396
-2.745    0.398    3.320
-3.396    3.320    -6.513
24.812    2.476    7.218
2.476    21.828    -4.046
7.218    -4.046    37.739

```

```

orbtensor 24 H
-4.701    -8.223    1.800
-8.223    -4.738    3.597
1.800    3.597    0.140
30.992    11.788    -0.412
11.788    30.038    -3.939
-0.412    -3.939    24.445

```

```

orbtensor 25 H
-13.016    4.356    -3.999
4.356    2.017    -0.721
-3.999    -0.721    0.035
40.593    -6.440    3.185
-6.440    20.451    1.540
3.185    1.540    24.366

```

```

gtensor (ppt)
0.00 0.00 0.00
0.00 0.00 0.00
0.00 0.00 0.00
0.00 0.00 0.00
0.00 0.00 0.00
0.00 0.00 0.00

```

```

averaging
Cis Average:3,20,23
Trans Average:2,24,25

```

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4610	25.03367	-97.73541	-0.00000	-97.73541	-72.70174
3	H	0.0020	24.74100	-0.42401	0.00000	-0.42401	24.31699
4	H	0.5533	27.80033	-117.31076	0.00000	-117.31076	-89.51043
5	H	0.1233	28.58900	-26.14758	0.00000	-26.14758	2.44142
6	H	0.0993	29.30800	-21.05940	0.00000	-21.05940	8.24860
7	H	0.3110	28.33300	-65.93430	0.00000	-65.93430	-37.60130
8	H	0.1503	27.24100	-31.87178	0.00000	-31.87178	-4.63078
9	H	0.8087	29.88367	-171.44332	0.00000	-171.44332	-141.55965
10	H	0.0790	29.46067	-16.74858	0.00000	-16.74858	12.71208
11	H	-0.0683	27.62900	14.48717	-0.00000	14.48717	42.11617
12	H	0.9567	28.47267	-202.82041	0.00000	-202.82041	-174.34775
13	H	-0.1313	27.09433	27.84364	0.00000	27.84364	54.93797
14	H	0.1257	30.18167	-26.64226	0.00000	-26.64226	3.53940
15	H	0.2723	28.82133	-57.73668	0.00000	-57.73668	-28.91535

16	H	1.0047	28.55967	-212.99677	0.00000	-212.99677	-184.43710
17	H	0.3527	29.20533	-74.76794	-0.00000	-74.76794	-45.56261
18	H	0.2167	27.60800	-45.93494	0.00000	-45.93494	-18.32694
19	H	0.3690	27.33067	-78.23073	0.00000	-78.23073	-50.90006
20	H	-0.0287	24.80433	6.07755	-0.00000	6.07755	30.88188
21	H	-0.1880	26.97333	39.85739	0.00000	39.85739	66.83072
22	H	-0.0123	26.80100	2.61476	-0.00000	2.61476	29.41576
23	H	-0.0727	25.37900	15.40587	0.00000	15.40587	40.78487
24	H	0.3760	25.39200	-79.71478	-0.00000	-79.71478	-54.32278
25	H	0.4283	24.81533	-90.80984	0.00000	-90.80984	-65.99450
Cis Average		-0.0331	24.97478	7.01980	0.00000	7.01980	31.99458
Trans Average		0.4218	25.08033	-89.42001	-0.00000	-89.42001	-64.33968

=====
FeL3-STO-PBE0-No-PSOSO

Temperature: 298

Spin: 2

atensor 2 H

-0.192 -0.112 0.010
-0.112 1.678 -0.370
0.010 -0.370 -0.116
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 H

-0.842 0.160 -0.103
0.160 0.963 -1.094
-0.103 -1.094 -0.128
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 H

-0.681 -0.323 -0.105
-0.323 2.648 0.997
-0.105 0.997 -0.310
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 H

-1.341 0.179 -0.532
0.179 -1.037 -1.338
-0.532 -1.338 2.768
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H

-1.301 -0.224 -0.855
-0.224 -1.108 1.161
-0.855 1.161 2.750
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 H

-0.769 0.515 -0.521
0.515 0.825 -1.845
-0.521 -1.845 0.875
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-1.567 -2.226 1.086
-2.226 3.204 -2.642
1.086 -2.642 -1.230
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 H
-0.057 0.664 0.811
0.664 1.099 1.694
0.810 1.694 1.423
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-0.963 0.052 1.447
0.052 -1.452 0.249
1.447 0.249 2.699
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 H
-0.739 2.450 -0.454
2.450 2.415 -0.844
-0.454 -0.844 -1.886
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
0.353 -0.808 1.073
-0.808 0.881 -1.537
1.073 -1.537 1.631
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 H
-0.546 -2.553 -0.495
-2.553 2.027 0.847
-0.495 0.847 -1.907
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
0.167 3.206 1.668
3.206 1.591 2.162
1.668 2.162 -1.328
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 H
-0.090 -0.930 -1.304
-0.930 0.058 1.379
-1.304 1.379 0.856
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 H
1.481 0.161 -1.864
0.161 -0.169 -0.149

-1.864 -0.149 1.699
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 H
0.940 0.450 1.827
0.450 -0.744 0.485
1.827 0.485 0.883
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 H
3.929 -0.981 -2.841
-0.981 -2.201 0.398
-2.840 0.398 -1.112
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 H
1.311 1.602 -0.822
1.602 0.262 -0.622
-0.822 -0.622 -0.481
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 H
0.311 -0.883 -0.918
-0.883 -0.289 0.682
-0.918 0.682 -0.119
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H
3.438 0.180 0.949
0.180 -2.118 0.033
0.949 0.033 -1.916
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 22 H
1.520 -1.268 0.932
-1.268 -0.718 -0.397
0.932 -0.397 -0.872
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 H
0.617 0.652 1.010
0.652 -0.654 0.402
1.010 0.402 -0.172
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 H
1.049 0.901 0.265
0.901 0.315 0.177
0.265 0.177 -0.237
0.000 0.000 0.000
0.000 0.000 0.000

0.000 0.000 0.000

atensor 25 H
1.332 -0.752 -0.328
-0.752 0.114 0.168
-0.328 0.168 -0.180
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 2 H
2.618 3.772 2.100
3.772 -12.573 -3.389
2.100 -3.389 -0.691
19.493 -4.594 -2.859
-4.594 41.394 2.714
-2.859 2.714 24.860

orbtensor 3 H
2.765 0.436 3.987
0.436 -4.759 1.385
3.987 1.385 -8.208
19.739 0.009 -6.298
0.009 26.169 -3.951
-6.298 -3.951 38.517

orbtensor 4 H
4.331 -0.275 -0.315
-0.275 -6.695 -6.143
-0.315 -6.143 1.296
20.961 0.631 0.655
0.631 36.473 4.079
0.655 4.079 27.035

orbtensor 5 H
5.416 -0.672 1.484
-0.672 1.564 -0.448
1.484 -0.448 -5.348
24.542 -0.921 0.098
-0.921 25.493 1.913
0.098 1.913 34.100

orbtensor 6 H
2.684 0.522 -0.946
0.522 4.843 -0.888
-0.946 -0.888 -3.898
26.192 -0.001 1.734
-0.001 24.057 -1.078
1.734 -1.078 34.046

orbtensor 7 H
5.190 -3.141 0.721
-3.141 -3.344 3.315
0.721 3.315 0.710
24.840 3.394 0.038
3.394 32.616 -6.202
0.038 -6.202 24.987

orbtensor 8 H
4.984 5.752 -2.704
5.752 -7.178 2.611
-2.704 2.611 -2.454
25.658 -0.428 -2.501
-0.428 32.780 2.484
-2.501 2.484 27.933

orbtensor 9 H

5.914	-0.911	-0.731
-0.911	2.499	-4.861
-0.731	-4.861	-1.337
23.749	1.198	3.373
1.198	29.242	7.479
3.373	7.479	29.584

orbtensor 10 H

3.804	-1.506	-0.206
-1.506	4.149	2.225
-0.206	2.225	-3.781
24.519	0.850	-1.727
0.850	25.552	-0.787
-1.727	-0.787	34.139

orbtensor 11 H

2.172	-2.024	0.945
-2.024	-8.164	3.443
0.945	3.443	2.265
26.384	-2.146	2.341
-2.146	35.753	0.935
2.341	0.935	24.477

orbtensor 12 H

3.564	2.126	-4.832
2.126	2.310	3.752
-4.832	3.752	-3.071
26.695	-2.801	4.835
-2.801	25.914	-6.637
4.835	-6.637	30.006

orbtensor 13 H

-5.447	5.573	2.177
5.573	-2.940	-2.477
2.177	-2.477	3.099
35.155	-3.160	-0.838
-3.160	26.821	-2.376
-0.838	-2.376	24.595

orbtensor 14 H

3.673	-6.512	-0.759
-6.512	0.428	-1.453
-0.759	-1.453	0.069
30.649	3.107	-1.084
3.107	27.815	-3.437
-1.084	-3.437	27.911

orbtensor 15 H

0.950	4.303	2.432
4.303	1.030	-2.679
2.432	-2.679	2.002
27.493	-5.030	-5.394
-5.030	29.735	3.162
-5.394	3.162	25.254

orbtensor 16 H

1.275	-1.665	5.547
-1.665	5.274	1.380
5.547	1.380	-3.247
28.364	1.764	-8.146
1.764	23.957	-0.923
-8.146	-0.923	30.056

orbtensor 17 H

-2.649	-1.684	-3.056
-1.684	5.336	-0.397
-3.056	-0.397	2.313

33.601	1.753	5.321
1.753	23.951	3.155
5.321	3.155	25.064

orbtensor 18 H

-8.731	1.536	3.132
1.536	6.856	-2.078
3.132	-2.078	-1.619
31.330	-2.833	3.378
-2.833	27.087	0.964
3.378	0.964	27.901

orbtensor 19 H

-4.398	-5.014	6.189
-5.014	1.893	3.008
6.189	3.008	0.075
32.890	6.516	-3.854
6.516	24.415	-1.796
-3.854	-1.796	27.117

orbtensor 20 H

-3.797	2.432	-1.058
2.432	1.233	-4.714
-1.058	-4.714	-7.298
24.641	-2.404	0.084
-2.404	21.356	7.786
0.084	7.786	38.278

orbtensor 21 H

-8.317	-2.926	-2.950
-2.926	0.208	-1.942
-2.950	-1.942	2.550
31.700	5.259	-1.757
5.259	30.191	1.864
-1.757	1.864	24.588

orbtensor 22 H

-4.415	5.586	-5.877
5.586	0.082	2.996
-5.877	2.996	0.532
31.881	-7.026	3.306
-7.026	25.374	-2.597
3.306	-2.597	26.949

orbtensor 23 H

-2.127	-2.745	-3.396
-2.745	0.398	3.320
-3.396	3.320	-6.513
24.812	2.476	7.218
2.476	21.828	-4.046
7.218	-4.046	37.739

orbtensor 24 H

-4.701	-8.223	1.800
-8.223	-4.738	3.597
1.800	3.597	0.140
30.992	11.788	-0.412
11.788	30.038	-3.939
-0.412	-3.939	24.445

orbtensor 25 H

-13.016	4.356	-3.999
4.356	2.017	-0.721
-3.999	-0.721	0.035
40.593	-6.440	3.185
-6.440	20.451	1.540
3.185	1.540	24.366

gtensor (ppt)
 0.00 0.00 0.00
 0.00 0.00 0.00
 0.00 0.00 0.00
 0.00 0.00 0.00
 0.00 0.00 0.00
 0.00 0.00 0.00

averaging
 Cis Average:3,20,23
 Trans Average:2,24,25

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4567	25.03367	-96.81671	-0.00000	-96.81671	-71.78305
3	H	-0.0023	24.74100	0.49468	0.00000	0.49468	25.23568
4	H	0.5523	27.80033	-117.09875	-0.00000	-117.09875	-89.29842
5	H	0.1300	28.58900	-27.56096	-0.00000	-27.56096	1.02804
6	H	0.1137	29.30800	-24.09817	0.00000	-24.09817	5.20983
7	H	0.3103	28.33300	-65.79296	0.00000	-65.79296	-37.45996
8	H	0.1357	27.24100	-28.76234	0.00000	-28.76234	-1.52134
9	H	0.8217	29.88367	-174.19941	0.00000	-174.19941	-144.31575
10	H	0.0947	29.46067	-20.07003	-0.00000	-20.07003	9.39063
11	H	-0.0700	27.62900	14.84052	0.00000	14.84052	42.46952
12	H	0.9550	28.47267	-202.46707	0.00000	-202.46707	-173.99440
13	H	-0.1420	27.09433	30.10505	0.00000	30.10505	57.19938
14	H	0.1433	30.18167	-30.38773	0.00000	-30.38773	-0.20606
15	H	0.2747	28.82133	-58.23137	0.00000	-58.23137	-29.41003
16	H	1.0037	28.55967	-212.78476	0.00000	-212.78476	-184.22509
17	H	0.3597	29.20533	-76.25199	-0.00000	-76.25199	-47.04666
18	H	0.2053	27.60800	-43.53219	0.00000	-43.53219	-15.92419
19	H	0.3640	27.33067	-77.17069	0.00000	-77.17069	-49.84003
20	H	-0.0323	24.80433	6.85491	-0.00000	6.85491	31.65924
21	H	-0.1987	26.97333	42.11880	0.00000	42.11880	69.09214
22	H	-0.0233	26.80100	4.94684	-0.00000	4.94684	31.74784
23	H	-0.0697	25.37900	14.76985	0.00000	14.76985	40.14885
24	H	0.3757	25.39200	-79.64411	-0.00000	-79.64411	-54.25211
25	H	0.4220	24.81533	-89.46712	0.00000	-89.46712	-64.65179
Cis Average		-0.0348	24.97478	7.37315	0.00000	7.37315	32.34792
Trans Average		0.4181	25.08033	-88.64265	-0.00000	-88.64265	-63.56232

=====
 FeL3-STO-PBE0-No-ZORA
 Temperature: 298
 Spin: 2

atensor 2 H
 -0.195 -0.113 0.010
 -0.113 1.677 -0.369
 0.010 -0.369 -0.118
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

atensor 3 H
 -0.845 0.160 -0.104
 0.160 0.961 -1.095
 -0.104 -1.095 -0.129
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

atensor 4 H
-0.644 -0.323 -0.104
-0.323 2.685 0.996
-0.104 0.996 -0.273
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 H
-1.337 0.179 -0.530
0.179 -1.034 -1.338
-0.530 -1.338 2.771
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H
-1.298 -0.224 -0.856
-0.224 -1.104 1.160
-0.856 1.160 2.754
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 H
-0.752 0.515 -0.520
0.515 0.842 -1.845
-0.520 -1.845 0.891
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-1.566 -2.223 1.083
-2.223 3.201 -2.639
1.083 -2.639 -1.229
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 H
-0.047 0.665 0.811
0.665 1.108 1.693
0.811 1.693 1.431
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-0.957 0.051 1.446
0.051 -1.447 0.251
1.446 0.251 2.703
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 H
-0.737 2.447 -0.454
2.447 2.419 -0.840
-0.454 -0.840 -1.880
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
0.360 -0.808 1.073

-0.808 0.889 -1.537
1.073 -1.537 1.638
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 H
-0.536 -2.552 -0.493
-2.552 2.029 0.844
-0.493 0.844 -1.897
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
0.171 3.203 1.667
3.203 1.589 2.158
1.667 2.158 -1.327
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 H
-0.067 -0.930 -1.304
-0.930 0.079 1.377
-1.304 1.377 0.877
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 H
1.491 0.160 -1.864
0.160 -0.159 -0.148
-1.864 -0.148 1.708
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 H
0.958 0.451 1.826
0.451 -0.726 0.485
1.826 0.485 0.900
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 H
3.924 -0.982 -2.835
-0.982 -2.197 0.398
-2.835 0.398 -1.113
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 H
1.359 1.602 -0.822
1.602 0.309 -0.621
-0.822 -0.621 -0.434
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 H
0.309 -0.883 -0.919
-0.883 -0.293 0.683
-0.919 0.683 -0.120
0.000 0.000 0.000

0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H
3.445 0.183 0.946
0.183 -2.107 0.032
0.946 0.032 -1.903
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 22 H
1.563 -1.268 0.931
-1.268 -0.675 -0.397
0.931 -0.397 -0.828
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 H
0.616 0.653 1.011
0.653 -0.655 0.402
1.011 0.402 -0.173
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 H
1.047 0.902 0.265
0.902 0.313 0.177
0.265 0.177 -0.238
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 H
1.332 -0.753 -0.327
-0.753 0.112 0.167
-0.327 0.167 -0.181
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 2 H
2.641 3.779 2.087
3.779 -12.612 -3.376
2.087 -3.376 -0.669
19.501 -4.597 -2.859
-4.597 41.409 2.713
-2.859 2.713 24.868

orbtensor 3 H
2.793 0.424 3.994
0.424 -4.789 1.433
3.994 1.433 -8.229
19.746 0.010 -6.300
0.010 26.175 -3.955
-6.300 -3.955 38.534

orbtensor 4 H
4.368 -0.271 -0.329
-0.271 -6.732 -6.165
-0.329 -6.165 1.343
20.965 0.631 0.658
0.631 36.485 4.079
0.658 4.079 27.042

orbtensor 5 H
5.456 -0.686 1.504
-0.686 1.571 -0.401
1.504 -0.401 -5.460
24.558 -0.925 0.097
-0.925 25.509 1.918
0.097 1.918 34.109

orbtensor 6 H
2.717 0.523 -0.921
0.523 4.886 -0.917
-0.921 -0.917 -3.973
26.211 0.001 1.739
0.001 24.069 -1.080
1.739 -1.080 34.055

orbtensor 7 H
5.217 -3.159 0.736
-3.159 -3.375 3.373
0.736 3.373 0.674
24.854 3.395 0.035
3.395 32.630 -6.202
0.035 -6.202 24.993

orbtensor 8 H
5.020 5.812 -2.748
5.812 -7.306 2.696
-2.748 2.696 -2.434
25.676 -0.424 -2.510
-0.424 32.791 2.494
-2.510 2.494 27.944

orbtensor 9 H
5.936 -0.917 -0.751
-0.917 2.515 -4.897
-0.751 -4.897 -1.334
23.761 1.198 3.376
1.198 29.258 7.479
3.376 7.479 29.591

orbtensor 10 H
3.836 -1.502 -0.250
-1.502 4.188 2.230
-0.250 2.230 -3.857
24.531 0.851 -1.731
0.851 25.571 -0.789
-1.731 -0.789 34.147

orbtensor 11 H
2.191 -2.072 0.973
-2.072 -8.235 3.461
0.973 3.461 2.315
26.392 -2.153 2.344
-2.153 35.766 0.943
2.344 0.943 24.485

orbtensor 12 H
3.576 2.147 -4.864
2.147 2.286 3.798
-4.864 3.798 -3.112
26.708 -2.803 4.834
-2.803 25.928 -6.639
4.834 -6.639 30.015

orbtensor 13 H
-5.468 5.634 2.173
5.634 -2.975 -2.504

2.173	-2.504	3.173
35.170	-3.158	-0.833
-3.158	26.825	-2.381
-0.833	-2.381	24.601

orbtensor 14 H

3.670	-6.579	-0.791
-6.579	0.417	-1.498
-0.791	-1.498	0.146
30.668	3.101	-1.088
3.101	27.827	-3.451
-1.088	-3.451	27.921

orbtensor 15 H

0.951	4.318	2.470
4.318	1.049	-2.719
2.470	-2.719	1.998
27.506	-5.030	-5.392
-5.030	29.750	3.164
-5.392	3.164	25.260

orbtensor 16 H

1.258	-1.679	5.608
-1.679	5.292	1.377
5.608	1.377	-3.289
28.379	1.765	-8.148
1.765	23.970	-0.921
-8.148	-0.921	30.065

orbtensor 17 H

-2.656	-1.684	-3.103
-1.684	5.364	-0.415
-3.103	-0.415	2.318
33.616	1.751	5.322
1.751	23.964	3.153
5.322	3.153	25.069

orbtensor 18 H

-8.861	1.548	3.218
1.548	6.906	-2.129
3.218	-2.129	-1.577
31.338	-2.832	3.391
-2.832	27.106	0.967
3.391	0.967	27.911

orbtensor 19 H

-4.431	-5.062	6.237
-5.062	1.899	3.015
6.237	3.015	0.090
32.898	6.520	-3.854
6.520	24.421	-1.795
-3.854	-1.795	27.124

orbtensor 20 H

-3.797	2.454	-1.027
2.454	1.250	-4.740
-1.027	-4.740	-7.278
24.645	-2.404	0.081
-2.404	21.362	7.790
0.081	7.790	38.295

orbtensor 21 H

-8.407	-2.936	-2.978
-2.936	0.226	-1.959
-2.978	-1.959	2.611
31.705	5.264	-1.765
5.264	30.204	1.863

-1.765 1.863 24.594

orbtensor 22 H

-4.451 5.635 -5.910
5.635 0.085 3.009
-5.910 3.009 0.560
31.891 -7.029 3.305
-7.029 25.378 -2.598
3.305 -2.598 26.957

orbtensor 23 H

-2.140 -2.752 -3.430
-2.752 0.429 3.304
-3.430 3.304 -6.499
24.819 2.475 7.224
2.475 21.835 -4.046
7.224 -4.046 37.756

orbtensor 24 H

-4.716 -8.249 1.797
-8.249 -4.734 3.580
1.797 3.580 0.170
31.003 11.793 -0.411
11.793 30.051 -3.938
-0.411 -3.938 24.454

orbtensor 25 H

-13.046 4.377 -3.982
4.377 2.032 -0.725
-3.982 -0.725 0.065
40.608 -6.442 3.183
-6.442 20.458 1.541
3.183 1.541 24.373

gtensor (ppt)

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

averaging

Cis Average:3,20,23

Trans Average:2,24,25

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4547	25.04600	-96.39270	-0.00000	-96.39270	-71.34670
3	H	-0.0043	24.74333	0.91870	0.00000	0.91870	25.66203
4	H	0.5893	27.82367	-124.94303	-0.00000	-124.94303	-97.11936
5	H	0.1333	28.58100	-28.26765	0.00000	-28.26765	0.31335
6	H	0.1173	29.32167	-24.87553	0.00000	-24.87553	4.44613
7	H	0.3270	28.33100	-69.32642	-0.00000	-69.32642	-40.99542
8	H	0.1353	27.23033	-28.69167	0.00000	-28.69167	-1.46133
9	H	0.8307	29.90900	-176.10748	-0.00000	-176.10748	-146.19848
10	H	0.0997	29.47200	-21.13007	0.00000	-21.13007	8.34193
11	H	-0.0660	27.63800	13.99249	0.00000	13.99249	41.63049
12	H	0.9623	28.46700	-204.02179	0.00000	-204.02179	-175.55479
13	H	-0.1347	27.10867	28.55033	0.00000	28.55033	55.65900
14	H	0.1443	30.21633	-30.59973	0.00000	-30.59973	-0.38340
15	H	0.2963	28.83800	-62.82486	0.00000	-62.82486	-33.98686
16	H	1.0133	28.55833	-214.83417	0.00000	-214.83417	-186.27583
17	H	0.3773	29.22500	-79.99746	0.00000	-79.99746	-50.77246

18	H	0.2047	27.60767	-43.39085	0.00000	-43.39085	-15.78318
19	H	0.4113	27.33367	-87.20571	0.00000	-87.20571	-59.87204
20	H	-0.0347	24.82567	7.34959	-0.00000	7.34959	32.17526
21	H	-0.1883	26.97767	39.92806	-0.00000	39.92806	66.90573
22	H	0.0200	26.80667	-4.24015	0.00000	-4.24015	22.56652
23	H	-0.0707	25.40000	14.98186	0.00000	14.98186	40.38186
24	H	0.3740	25.40933	-79.29077	-0.00000	-79.29077	-53.88143
25	H	0.4210	24.83000	-89.25512	0.00000	-89.25512	-64.42512
	Cis Average	-0.0366	24.98967	7.75005	0.00000	7.75005	32.73971
	Trans Average	0.4166	25.09511	-88.31286	-0.00000	-88.31286	-63.21775

=====

FeL4-STO-PBE0-Full

Temperature: 298

Spin: 2

atensor 2 H

-0.333 0.253 0.258
0.253 0.931 1.741
0.258 1.741 1.746
-0.040 -0.008 -0.010
0.006 -0.013 0.016
0.015 0.046 0.011

atensor 3 H

-0.203 -0.036 -0.038
-0.036 0.031 0.369
-0.038 0.369 0.368
-0.008 -0.003 -0.005
0.001 -0.004 0.003
0.001 0.011 0.006

atensor 4 H

-0.411 -0.035 0.022
-0.035 0.853 -0.743
0.022 -0.743 -0.004
-0.019 0.000 0.005
0.003 0.018 -0.011
0.004 -0.027 0.003

atensor 5 H

-2.267 0.017 -0.316
0.017 -2.011 -1.069
-0.316 -1.069 4.379
-0.072 0.024 -0.037
0.019 -0.027 -0.052
0.003 -0.011 0.134

atensor 6 H

-1.059 0.891 2.479
0.891 -1.660 1.954
2.479 1.954 2.945
-0.068 0.025 0.044
0.000 -0.050 -0.006
0.073 0.067 0.050

atensor 7 H

-0.659 -0.770 -0.423
-0.770 1.213 1.155
-0.423 1.155 -0.277
-0.016 -0.038 -0.018
-0.004 0.011 0.024
-0.002 0.030 -0.019

atensor 8 H

-0.336 -0.185 -0.220

-0.185 0.093 0.576
-0.220 0.576 0.265
-0.008 -0.010 -0.011
0.000 -0.003 0.007
-0.002 0.017 0.004

atensor 9 H
-1.670 -1.361 1.348
-1.361 1.009 -3.441
1.348 -3.441 1.197
-0.067 -0.029 0.061
-0.021 0.050 -0.071
0.064 -0.092 0.048

atensor 10 H
-1.780 1.915 0.094
1.915 4.427 0.588
0.094 0.588 -2.300
-0.073 0.045 0.020
0.042 0.053 0.031
0.001 -0.038 -0.079

atensor 11 H
-0.294 0.442 0.235
0.442 0.747 0.660
0.235 0.660 -0.098
-0.017 0.006 0.006
0.007 0.003 0.011
0.006 0.009 -0.015

atensor 12 H
0.196 -3.900 -2.083
-3.900 1.498 2.504
-2.083 2.504 -1.627
0.046 -0.143 -0.075
-0.042 0.018 0.075
-0.035 0.084 -0.068

atensor 13 H
-1.455 -2.259 0.206
-2.259 3.715 -0.461
0.206 -0.461 -2.290
-0.040 -0.096 0.024
-0.029 0.076 0.011
0.037 -0.030 -0.062

atensor 14 H
0.434 1.339 -4.329
1.339 -2.573 -1.550
-4.329 -1.550 2.190
0.036 0.058 -0.137
0.052 -0.035 -0.025
-0.132 -0.029 0.103

atensor 15 H
-0.622 0.695 -0.975
0.695 -0.379 -1.183
-0.975 -1.183 0.504
-0.011 0.030 -0.031
0.021 0.003 -0.018
-0.029 -0.035 0.036

atensor 16 H
-0.452 0.111 0.246
0.111 -0.437 0.296
0.246 0.296 0.468
-0.011 0.002 0.002

0.001 -0.007 -0.002
0.008 0.009 0.012

atensor 17 H
-0.046 -0.118 -1.217
-0.118 -0.417 0.344
-1.217 0.344 2.428
-0.011 -0.001 -0.052
0.012 -0.019 -0.001
-0.027 0.019 0.053

atensor 18 H
-0.205 -1.115 -0.719
-1.115 1.306 1.409
-0.719 1.409 0.184
-0.009 -0.051 -0.030
-0.006 0.007 0.029
-0.009 0.041 -0.012

atensor 19 H
0.344 1.195 -0.469
1.195 2.454 -1.010
-0.469 -1.010 0.093
-0.024 0.040 -0.005
0.029 0.024 -0.006
-0.021 -0.049 -0.010

atensor 20 H
-0.218 -0.288 0.227
-0.288 0.164 -0.425
0.227 -0.425 -0.034
-0.006 -0.008 0.009
-0.005 0.008 -0.008
0.010 -0.012 0.003

atensor 21 H
0.030 -0.864 -0.965
-0.864 -0.014 0.950
-0.965 0.950 0.213
0.010 -0.031 -0.037
-0.004 -0.005 0.018
-0.021 0.033 0.002

atensor 22 H
-0.068 0.408 0.015
0.408 0.512 0.067
0.015 0.067 -0.228
-0.006 0.011 0.004
0.007 0.005 0.004
-0.002 -0.005 -0.010

atensor 23 H
0.161 0.880 -1.394
0.880 -0.066 -1.165
-1.394 -1.165 1.066
0.000 0.039 -0.043
0.026 -0.003 -0.016
-0.045 -0.034 0.037

atensor 24 H
5.479 0.492 1.608
0.492 -2.833 0.050
1.608 0.050 -2.614
0.165 0.035 0.060
-0.033 -0.061 0.021
0.000 0.036 -0.087

atensor 25 H
-0.003 -0.051 0.712
-0.051 -0.352 -0.049
0.712 -0.049 1.016
-0.011 0.003 0.018
-0.005 -0.008 -0.012
0.022 0.002 0.019

atensor 26 H
1.699 3.021 1.885
3.021 -0.190 1.365
1.885 1.365 -1.389
0.026 0.090 0.067
0.024 -0.031 0.026
0.015 0.020 -0.075

atensor 27 H
1.328 -0.979 1.472
-0.979 0.502 -0.999
1.472 -0.999 1.514
0.002 -0.021 0.053
-0.027 0.005 -0.028
0.046 -0.016 0.008

atensor 28 H
0.608 0.716 -1.152
0.716 -0.658 -0.519
-1.152 -0.519 -0.162
0.025 0.028 -0.033
0.018 -0.008 -0.002
-0.043 -0.013 0.010

atensor 29 H
1.010 -1.402 -1.663
-1.402 -0.541 1.013
-1.663 1.013 -0.131
0.046 -0.048 -0.060
-0.010 -0.010 0.028
-0.045 0.043 -0.004

atensor 30 H
0.036 0.466 -0.347
0.466 0.092 -0.352
-0.347 -0.352 -0.125
0.002 0.017 -0.008
0.010 0.002 -0.003
-0.014 -0.014 0.002

atensor 31 H
0.947 -1.749 0.041
-1.749 0.990 0.004
0.041 0.004 -0.755
0.029 -0.060 0.008
-0.030 0.020 0.010
0.012 0.004 -0.032

atensor 32 H
0.052 0.369 -0.118
0.369 0.306 -0.170
-0.118 -0.170 -0.157
-0.001 0.012 -0.002
0.007 0.003 0.000
-0.007 -0.009 -0.004

atensor 33 H
1.577 0.412 -2.043
0.412 -1.274 -0.268

-2.043 -0.268 0.052
0.059 0.024 -0.064
0.016 -0.022 0.007
-0.069 0.000 0.014

atensor 34 H
1.134 0.041 1.231
0.041 -1.078 0.021
1.231 0.021 -0.405
0.033 0.007 0.041
-0.017 -0.018 -0.004
0.026 0.010 -0.016

atensor 35 H
1.621 -0.550 0.398
-0.550 -0.724 -0.094
0.398 -0.094 -0.775
0.052 -0.013 0.017
-0.022 -0.009 0.005
0.007 0.009 -0.024

atensor 36 H
2.514 1.404 -0.086
1.404 0.340 -0.094
-0.086 -0.094 -0.324
0.047 0.048 0.004
0.014 -0.015 0.009
-0.028 -0.006 -0.031

atensor 37 H
2.906 -0.696 -0.482
-0.696 -1.235 0.046
-0.482 0.046 -1.287
0.098 -0.016 -0.006
-0.027 -0.018 0.019
-0.022 0.020 -0.040

atensor 38 H
2.390 -0.133 1.172
-0.133 -0.851 -0.081
1.172 -0.081 -0.452
0.060 0.002 0.045
-0.026 -0.018 -0.001
0.022 0.010 -0.029

atensor 39 H
0.153 -0.262 0.298
-0.262 -0.031 -0.216
0.298 -0.216 0.021
0.003 -0.007 0.011
-0.008 0.002 -0.005
0.010 -0.004 -0.001

orbtensor 2 H
5.100 1.082 2.357
1.082 1.744 -5.557
2.357 -5.557 -5.206
23.913 2.081 -1.833
2.081 28.612 6.894
-1.833 6.894 33.378

orbtensor 3 H
2.118 0.992 -1.373
0.992 -0.390 -4.019
-1.373 -4.019 -6.219
21.852 -2.703 3.743
-2.703 24.816 8.062

3.743 8.062 39.780

orbtensor 4 H

-5.509 -8.239 1.951
-8.239 -12.710 5.688
1.951 5.688 -1.744
31.812 6.537 0.259
6.537 35.033 -7.075
0.259 -7.075 24.471

orbtensor 5 H

5.006 -1.573 0.204
-1.573 5.027 4.167
0.204 4.167 -10.005
29.627 -3.651 2.024
-3.651 27.931 -1.938
2.024 -1.938 26.908

orbtensor 6 H

6.762 -0.082 -6.481
-0.082 1.964 1.222
-6.481 1.222 -5.325
28.247 -2.677 3.535
-2.677 30.650 -3.257
3.535 -3.257 26.629

orbtensor 7 H

2.852 2.691 0.046
2.691 -1.457 -1.733
0.046 -1.733 5.258
22.375 -1.387 0.948
-1.387 34.002 -0.666
0.948 -0.666 26.775

orbtensor 8 H

-3.536 4.082 -1.578
4.082 -1.202 -0.803
-1.578 -0.803 -0.381
32.923 -9.570 4.657
-9.570 27.301 2.714
4.657 2.714 27.623

orbtensor 9 H

6.825 -0.228 -5.917
-0.228 -9.622 6.020
-5.917 6.020 -3.474
27.072 5.122 0.108
5.122 31.573 -0.339
0.108 -0.339 26.833

orbtensor 10 H

7.383 -3.886 -3.258
-3.886 -3.199 -1.203
-3.258 -1.203 2.336
24.098 -0.787 1.139
-0.787 27.510 2.592
1.139 2.592 34.049

orbtensor 11 H

1.234 -0.298 1.104
-0.298 -5.493 -8.687
1.104 -8.687 -12.573
22.737 3.167 -2.937
3.167 32.030 7.321
-2.937 7.321 36.537

orbtensor 12 H

-3.471	10.395	3.944
10.395	-1.179	-7.435
3.944	-7.435	7.421
23.184	-3.177	2.236
-3.177	23.306	4.420
2.236	4.420	35.416

orbtensor 13 H

4.763	4.424	-0.374
4.424	-6.194	1.643
-0.374	1.643	6.549
29.427	3.755	-1.165
3.755	29.637	-1.087
-1.165	-1.087	25.291

orbtensor 14 H

-0.887	-6.021	13.156
-6.021	4.010	1.358
13.156	1.358	-10.018
25.854	7.787	-2.365
7.787	31.803	1.871
-2.365	1.871	24.698

orbtensor 15 H

4.436	-1.398	2.680
-1.398	1.892	2.467
2.680	2.467	-4.135
23.733	1.704	1.884
1.704	26.267	-2.724
1.884	-2.724	32.997

orbtensor 16 H

-2.088	-1.454	-6.186
-1.454	-1.300	-4.171
-6.186	-4.171	-15.781
26.344	-1.879	6.836
-1.879	26.320	5.223
6.836	5.223	38.717

orbtensor 17 H

2.265	0.555	6.400
0.555	4.027	-2.246
6.400	-2.246	-5.230
24.073	-0.713	-5.916
-0.713	24.687	2.740
-5.916	2.740	34.755

orbtensor 18 H

2.993	1.653	1.521
1.653	-1.319	-5.255
1.521	-5.255	2.841
24.962	-1.701	-0.240
-1.701	32.297	6.201
-0.240	6.201	25.384

orbtensor 19 H

-0.915	-6.997	2.811
-6.997	-2.630	4.030
2.811	4.030	1.998
29.619	5.041	-1.415
5.041	32.986	-5.109
-1.415	-5.109	23.266

orbtensor 20 H

-1.618	3.759	-3.814
3.759	-11.187	8.901
-3.814	8.901	-7.430

28.575	-1.727	4.319
-1.727	34.014	-9.889
4.319	-9.889	28.790

orbtensor 21 H

-0.810	3.092	3.653
3.092	2.825	-1.578
3.653	-1.578	2.040
32.727	-2.461	-3.814
-2.461	22.632	1.425
-3.814	1.425	27.370

orbtensor 22 H

-2.012	-6.329	-0.786
-6.329	-16.093	-2.402
-0.786	-2.402	-0.503
24.390	7.354	-1.556
7.354	39.498	2.945
-1.556	2.945	27.532

orbtensor 23 H

2.701	-3.203	4.420
-3.203	-0.306	4.517
4.420	4.517	-2.020
23.997	1.809	-4.077
1.809	29.321	-5.435
-4.077	-5.435	29.228

orbtensor 24 H

-15.413	-1.328	-3.297
-1.328	5.956	-1.732
-3.297	-1.732	9.920
28.573	-3.447	3.839
-3.447	29.908	-7.020
3.839	-7.020	23.308

orbtensor 25 H

-8.310	7.027	-8.198
7.027	-4.500	4.538
-8.198	4.538	-6.744
30.891	-7.813	7.529
-7.813	28.312	-0.939
7.529	-0.939	32.016

orbtensor 26 H

-1.028	-3.416	-3.005
-3.416	4.378	-4.492
-3.005	-4.492	7.519
25.904	-0.336	-1.210
-0.336	26.443	3.174
-1.210	3.174	32.191

orbtensor 27 H

-4.115	5.928	-6.499
5.928	-1.051	2.813
-6.499	2.813	0.760
30.019	-6.297	5.336
-6.297	25.865	-2.062
5.336	-2.062	30.004

orbtensor 28 H

-1.883	-1.926	4.558
-1.926	4.227	-0.402
4.558	-0.402	-0.290
32.977	-0.142	-4.845
-0.142	24.849	1.708
-4.845	1.708	24.992

orbtensor 29 H
-6.004 0.007 7.224
0.007 1.640 -1.694
7.224 -1.694 0.939
33.151 0.110 -4.445
0.110 25.391 -1.021
-4.445 -1.021 26.085

orbtensor 30 H
0.575 -0.676 3.733
-0.676 -1.548 -1.993
3.733 -1.993 -5.072
23.465 1.909 -8.236
1.909 29.690 5.195
-8.236 5.195 34.683

orbtensor 31 H
-4.912 6.631 -0.922
6.631 -0.246 -0.824
-0.922 -0.824 5.928
31.417 -7.666 1.661
-7.666 28.939 0.413
1.661 0.413 23.241

orbtensor 32 H
0.393 -5.065 1.478
-5.065 -5.275 0.813
1.478 0.813 0.072
25.247 11.024 -2.907
11.024 36.789 0.387
-2.907 0.387 24.485

orbtensor 33 H
-9.103 0.206 4.588
0.206 3.422 -0.093
4.588 -0.093 0.719
34.126 -2.846 -1.991
-2.846 24.231 0.603
-1.991 0.603 26.254

orbtensor 34 H
-1.827 -1.817 -3.584
-1.817 3.272 -0.946
-3.584 -0.946 2.597
27.429 2.813 5.003
2.813 29.229 2.158
5.003 2.158 27.223

orbtensor 35 H
-4.984 1.079 0.194
1.079 2.360 -1.049
0.194 -1.049 5.549
33.038 -2.260 -3.941
-2.260 24.597 -0.916
-3.941 -0.916 24.516

orbtensor 36 H
-6.181 -4.614 2.965
-4.614 4.146 0.503
2.965 0.503 5.038
34.512 6.266 -0.978
6.266 25.660 -2.085
-0.978 -2.085 23.338

orbtensor 37 H
-8.084 3.745 3.575

```

3.745    1.771    -4.487
3.575   -4.487     2.146
31.201   -1.693   -4.762
-1.693   25.724     2.553
-4.762    2.553    27.531

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orbtensor 38 H
-4.678    1.374   -5.169
1.374    4.571   -0.244
-5.169   -0.244    1.908
32.085    0.430    5.584
0.430    21.919   -0.946
5.584   -0.946    28.507

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orbtensor 39 H
-2.308    2.346   -3.982
2.346   -1.886    4.455
-3.982    4.455   -1.183
28.544   -3.404    7.732
-3.404   28.930  -10.326
7.732  -10.326   28.912

```

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gtensor (ppt)
-0.196   -0.004    0.012
-0.004   -0.187    0.004
0.012    0.004   -0.204
63.517  -10.832  -13.092
-10.832   31.241  -17.121
-13.092  -17.121   55.545

```

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zfstensor (cm-1)
-1.243806  0.131563  1.554137
0.131563  1.022330  0.995550
1.554137  0.995550 -1.540924

```

averaging
NH2 Average:3,8,30,32,39

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.7673	29.18033	-166.75373	6.24190	-160.51183	-131.33150
3	H	0.0633	27.31900	-13.76334	0.74677	-13.01657	14.30243
4	H	0.1467	23.78433	-31.87300	0.05252	-31.82047	-8.03614
5	H	0.0453	28.16467	-9.85165	-9.53700	-19.38866	8.77601
6	H	0.0527	29.64233	-11.44530	9.54068	-1.90462	27.73771
7	H	0.0843	29.93500	-18.32697	4.15758	-14.16939	15.76561
8	H	0.0050	27.57600	-1.08658	0.89886	-0.18771	27.38829
9	H	0.1890	26.40233	-41.07270	-3.55666	-44.62936	-18.22703
10	H	0.0827	30.72567	-17.96478	15.85057	-2.11421	28.61146
11	H	0.1087	24.82400	-23.61499	4.74907	-18.86593	5.95807
12	H	0.0210	28.22567	-4.56363	0.30345	-4.26018	23.96548
13	H	-0.0187	29.82433	4.05656	7.88589	11.94245	41.76679
14	H	0.0517	25.15333	-11.22799	-24.64538	-35.87336	-10.72003
15	H	-0.1563	28.39667	33.97372	-6.36539	27.60833	56.00500
16	H	-0.1423	24.07067	30.93129	0.90045	31.83175	55.90242
17	H	0.6627	28.19233	-144.00800	-6.20974	-150.21774	-122.02540
18	H	0.4237	29.05267	-92.06950	2.84324	-89.22626	-60.17359
19	H	0.9603	28.10800	-208.69569	1.02343	-207.67226	-179.56426
20	H	-0.0277	23.71467	6.01241	-0.10122	5.91118	29.62585
21	H	0.0787	28.92800	-17.09552	-1.71777	-18.81329	10.11471
22	H	0.0683	24.27067	-14.84992	1.85093	-12.99899	11.27168
23	H	0.3983	27.64033	-86.56416	-8.22921	-94.79337	-67.15304
24	H	0.0163	27.41733	-3.54949	-2.30516	-5.85465	21.56268
25	H	0.2203	23.88833	-47.88193	0.60152	-47.28042	-23.39208

26	H	0.0133	31.80233	-2.89755	12.02885	9.13131	40.93364
27	H	1.1197	27.16067	-243.32136	-0.39550	-243.71686	-216.55619
28	H	-0.0617	28.29067	13.40115	-6.25524	7.14591	35.43658
29	H	0.1233	27.06733	-26.80229	-6.00126	-32.80355	-5.73622
30	H	0.0030	27.26433	-0.65195	-1.42202	-2.07397	25.19037
31	H	0.3997	28.12233	-86.85392	0.17401	-86.67991	-58.55758
32	H	0.0663	27.23700	-14.41529	0.15761	-14.25768	12.97932
33	H	0.1353	26.54967	-29.41008	-11.13187	-40.54195	-13.99228
34	H	-0.1167	29.30767	25.35352	1.43971	26.79323	56.10089
35	H	0.0470	28.35867	-10.21385	-1.65206	-11.86591	16.49276
36	H	0.8437	28.83767	-183.34217	-0.74551	-184.08768	-155.25001
37	H	0.1413	26.76300	-30.71398	-6.06975	-36.78373	-10.02073
38	H	0.3667	28.10400	-79.68249	0.07006	-79.61243	-51.50843
39	H	0.0490	27.00300	-10.64848	-0.05393	-10.70241	16.30059
NH2 Average		0.0373	27.27987	-8.11313	0.06546	-8.04767	19.23220

=====

FeL4-STO-PBE0-No-ZFS

Temperature: 298

Spin: 2

atensor 2 H

-0.333 0.253 0.258
0.253 0.931 1.741
0.258 1.741 1.746
-0.040 -0.008 -0.010
0.006 -0.013 0.016
0.015 0.046 0.011

atensor 3 H

-0.203 -0.036 -0.038
-0.036 0.031 0.369
-0.038 0.369 0.368
-0.008 -0.003 -0.005
0.001 -0.004 0.003
0.001 0.011 0.006

atensor 4 H

-0.411 -0.035 0.022
-0.035 0.853 -0.743
0.022 -0.743 -0.004
-0.019 0.000 0.005
0.003 0.018 -0.011
0.004 -0.027 0.003

atensor 5 H

-2.267 0.017 -0.316
0.017 -2.011 -1.069
-0.316 -1.069 4.379
-0.072 0.024 -0.037
0.019 -0.027 -0.052
0.003 -0.011 0.134

atensor 6 H

-1.059 0.891 2.479
0.891 -1.660 1.954
2.479 1.954 2.945
-0.068 0.025 0.044
0.000 -0.050 -0.006
0.073 0.067 0.050

atensor 7 H

-0.659 -0.770 -0.423
-0.770 1.213 1.155
-0.423 1.155 -0.277
-0.016 -0.038 -0.018

-0.004 0.011 0.024
-0.002 0.030 -0.019

atensor 8 H
-0.336 -0.185 -0.220
-0.185 0.093 0.576
-0.220 0.576 0.265
-0.008 -0.010 -0.011
0.000 -0.003 0.007
-0.002 0.017 0.004

atensor 9 H
-1.670 -1.361 1.348
-1.361 1.009 -3.441
1.348 -3.441 1.197
-0.067 -0.029 0.061
-0.021 0.050 -0.071
0.064 -0.092 0.048

atensor 10 H
-1.780 1.915 0.094
1.915 4.427 0.588
0.094 0.588 -2.300
-0.073 0.045 0.020
0.042 0.053 0.031
0.001 -0.038 -0.079

atensor 11 H
-0.294 0.442 0.235
0.442 0.747 0.660
0.235 0.660 -0.098
-0.017 0.006 0.006
0.007 0.003 0.011
0.006 0.009 -0.015

atensor 12 H
0.196 -3.900 -2.083
-3.900 1.498 2.504
-2.083 2.504 -1.627
0.046 -0.143 -0.075
-0.042 0.018 0.075
-0.035 0.084 -0.068

atensor 13 H
-1.455 -2.259 0.206
-2.259 3.715 -0.461
0.206 -0.461 -2.290
-0.040 -0.096 0.024
-0.029 0.076 0.011
0.037 -0.030 -0.062

atensor 14 H
0.434 1.339 -4.329
1.339 -2.573 -1.550
-4.329 -1.550 2.190
0.036 0.058 -0.137
0.052 -0.035 -0.025
-0.132 -0.029 0.103

atensor 15 H
-0.622 0.695 -0.975
0.695 -0.379 -1.183
-0.975 -1.183 0.504
-0.011 0.030 -0.031
0.021 0.003 -0.018
-0.029 -0.035 0.036

atensor 16 H
-0.452 0.111 0.246
0.111 -0.437 0.296
0.246 0.296 0.468
-0.011 0.002 0.002
0.001 -0.007 -0.002
0.008 0.009 0.012

atensor 17 H
-0.046 -0.118 -1.217
-0.118 -0.417 0.344
-1.217 0.344 2.428
-0.011 -0.001 -0.052
0.012 -0.019 -0.001
-0.027 0.019 0.053

atensor 18 H
-0.205 -1.115 -0.719
-1.115 1.306 1.409
-0.719 1.409 0.184
-0.009 -0.051 -0.030
-0.006 0.007 0.029
-0.009 0.041 -0.012

atensor 19 H
0.344 1.195 -0.469
1.195 2.454 -1.010
-0.469 -1.010 0.093
-0.024 0.040 -0.005
0.029 0.024 -0.006
-0.021 -0.049 -0.010

atensor 20 H
-0.218 -0.288 0.227
-0.288 0.164 -0.425
0.227 -0.425 -0.034
-0.006 -0.008 0.009
-0.005 0.008 -0.008
0.010 -0.012 0.003

atensor 21 H
0.030 -0.864 -0.965
-0.864 -0.014 0.950
-0.965 0.950 0.213
0.010 -0.031 -0.037
-0.004 -0.005 0.018
-0.021 0.033 0.002

atensor 22 H
-0.068 0.408 0.015
0.408 0.512 0.067
0.015 0.067 -0.228
-0.006 0.011 0.004
0.007 0.005 0.004
-0.002 -0.005 -0.010

atensor 23 H
0.161 0.880 -1.394
0.880 -0.066 -1.165
-1.394 -1.165 1.066
0.000 0.039 -0.043
0.026 -0.003 -0.016
-0.045 -0.034 0.037

atensor 24 H
5.479 0.492 1.608
0.492 -2.833 0.050

1.608 0.050 -2.614
0.165 0.035 0.060
-0.033 -0.061 0.021
0.000 0.036 -0.087

atensor 25 H
-0.003 -0.051 0.712
-0.051 -0.352 -0.049
0.712 -0.049 1.016
-0.011 0.003 0.018
-0.005 -0.008 -0.012
0.022 0.002 0.019

atensor 26 H
1.699 3.021 1.885
3.021 -0.190 1.365
1.885 1.365 -1.389
0.026 0.090 0.067
0.024 -0.031 0.026
0.015 0.020 -0.075

atensor 27 H
1.328 -0.979 1.472
-0.979 0.502 -0.999
1.472 -0.999 1.514
0.002 -0.021 0.053
-0.027 0.005 -0.028
0.046 -0.016 0.008

atensor 28 H
0.608 0.716 -1.152
0.716 -0.658 -0.519
-1.152 -0.519 -0.162
0.025 0.028 -0.033
0.018 -0.008 -0.002
-0.043 -0.013 0.010

atensor 29 H
1.010 -1.402 -1.663
-1.402 -0.541 1.013
-1.663 1.013 -0.131
0.046 -0.048 -0.060
-0.010 -0.010 0.028
-0.045 0.043 -0.004

atensor 30 H
0.036 0.466 -0.347
0.466 0.092 -0.352
-0.347 -0.352 -0.125
0.002 0.017 -0.008
0.010 0.002 -0.003
-0.014 -0.014 0.002

atensor 31 H
0.947 -1.749 0.041
-1.749 0.990 0.004
0.041 0.004 -0.755
0.029 -0.060 0.008
-0.030 0.020 0.010
0.012 0.004 -0.032

atensor 32 H
0.052 0.369 -0.118
0.369 0.306 -0.170
-0.118 -0.170 -0.157
-0.001 0.012 -0.002
0.007 0.003 0.000

-0.007 -0.009 -0.004

atensor 33 H
1.577 0.412 -2.043
0.412 -1.274 -0.268
-2.043 -0.268 0.052
0.059 0.024 -0.064
0.016 -0.022 0.007
-0.069 0.000 0.014

atensor 34 H
1.134 0.041 1.231
0.041 -1.078 0.021
1.231 0.021 -0.405
0.033 0.007 0.041
-0.017 -0.018 -0.004
0.026 0.010 -0.016

atensor 35 H
1.621 -0.550 0.398
-0.550 -0.724 -0.094
0.398 -0.094 -0.775
0.052 -0.013 0.017
-0.022 -0.009 0.005
0.007 0.009 -0.024

atensor 36 H
2.514 1.404 -0.086
1.404 0.340 -0.094
-0.086 -0.094 -0.324
0.047 0.048 0.004
0.014 -0.015 0.009
-0.028 -0.006 -0.031

atensor 37 H
2.906 -0.696 -0.482
-0.696 -1.235 0.046
-0.482 0.046 -1.287
0.098 -0.016 -0.006
-0.027 -0.018 0.019
-0.022 0.020 -0.040

atensor 38 H
2.390 -0.133 1.172
-0.133 -0.851 -0.081
1.172 -0.081 -0.452
0.060 0.002 0.045
-0.026 -0.018 -0.001
0.022 0.010 -0.029

atensor 39 H
0.153 -0.262 0.298
-0.262 -0.031 -0.216
0.298 -0.216 0.021
0.003 -0.007 0.011
-0.008 0.002 -0.005
0.010 -0.004 -0.001

orbtensor 2 H
5.100 1.082 2.357
1.082 1.744 -5.557
2.357 -5.557 -5.206
23.913 2.081 -1.833
2.081 28.612 6.894
-1.833 6.894 33.378

orbtensor 3 H

2.118	0.992	-1.373
0.992	-0.390	-4.019
-1.373	-4.019	-6.219
21.852	-2.703	3.743
-2.703	24.816	8.062
3.743	8.062	39.780

orbtensor 4 H

-5.509	-8.239	1.951
-8.239	-12.710	5.688
1.951	5.688	-1.744
31.812	6.537	0.259
6.537	35.033	-7.075
0.259	-7.075	24.471

orbtensor 5 H

5.006	-1.573	0.204
-1.573	5.027	4.167
0.204	4.167	-10.005
29.627	-3.651	2.024
-3.651	27.931	-1.938
2.024	-1.938	26.908

orbtensor 6 H

6.762	-0.082	-6.481
-0.082	1.964	1.222
-6.481	1.222	-5.325
28.247	-2.677	3.535
-2.677	30.650	-3.257
3.535	-3.257	26.629

orbtensor 7 H

2.852	2.691	0.046
2.691	-1.457	-1.733
0.046	-1.733	5.258
22.375	-1.387	0.948
-1.387	34.002	-0.666
0.948	-0.666	26.775

orbtensor 8 H

-3.536	4.082	-1.578
4.082	-1.202	-0.803
-1.578	-0.803	-0.381
32.923	-9.570	4.657
-9.570	27.301	2.714
4.657	2.714	27.623

orbtensor 9 H

6.825	-0.228	-5.917
-0.228	-9.622	6.020
-5.917	6.020	-3.474
27.072	5.122	0.108
5.122	31.573	-0.339
0.108	-0.339	26.833

orbtensor 10 H

7.383	-3.886	-3.258
-3.886	-3.199	-1.203
-3.258	-1.203	2.336
24.098	-0.787	1.139
-0.787	27.510	2.592
1.139	2.592	34.049

orbtensor 11 H

1.234	-0.298	1.104
-0.298	-5.493	-8.687
1.104	-8.687	-12.573

22.737	3.167	-2.937
3.167	32.030	7.321
-2.937	7.321	36.537

orbtensor 12 H

-3.471	10.395	3.944
10.395	-1.179	-7.435
3.944	-7.435	7.421
23.184	-3.177	2.236
-3.177	23.306	4.420
2.236	4.420	35.416

orbtensor 13 H

4.763	4.424	-0.374
4.424	-6.194	1.643
-0.374	1.643	6.549
29.427	3.755	-1.165
3.755	29.637	-1.087
-1.165	-1.087	25.291

orbtensor 14 H

-0.887	-6.021	13.156
-6.021	4.010	1.358
13.156	1.358	-10.018
25.854	7.787	-2.365
7.787	31.803	1.871
-2.365	1.871	24.698

orbtensor 15 H

4.436	-1.398	2.680
-1.398	1.892	2.467
2.680	2.467	-4.135
23.733	1.704	1.884
1.704	26.267	-2.724
1.884	-2.724	32.997

orbtensor 16 H

-2.088	-1.454	-6.186
-1.454	-1.300	-4.171
-6.186	-4.171	-15.781
26.344	-1.879	6.836
-1.879	26.320	5.223
6.836	5.223	38.717

orbtensor 17 H

2.265	0.555	6.400
0.555	4.027	-2.246
6.400	-2.246	-5.230
24.073	-0.713	-5.916
-0.713	24.687	2.740
-5.916	2.740	34.755

orbtensor 18 H

2.993	1.653	1.521
1.653	-1.319	-5.255
1.521	-5.255	2.841
24.962	-1.701	-0.240
-1.701	32.297	6.201
-0.240	6.201	25.384

orbtensor 19 H

-0.915	-6.997	2.811
-6.997	-2.630	4.030
2.811	4.030	1.998
29.619	5.041	-1.415
5.041	32.986	-5.109
-1.415	-5.109	23.266

orbtensor 20 H
-1.618 3.759 -3.814
3.759 -11.187 8.901
-3.814 8.901 -7.430
28.575 -1.727 4.319
-1.727 34.014 -9.889
4.319 -9.889 28.790

orbtensor 21 H
-0.810 3.092 3.653
3.092 2.825 -1.578
3.653 -1.578 2.040
32.727 -2.461 -3.814
-2.461 22.632 1.425
-3.814 1.425 27.370

orbtensor 22 H
-2.012 -6.329 -0.786
-6.329 -16.093 -2.402
-0.786 -2.402 -0.503
24.390 7.354 -1.556
7.354 39.498 2.945
-1.556 2.945 27.532

orbtensor 23 H
2.701 -3.203 4.420
-3.203 -0.306 4.517
4.420 4.517 -2.020
23.997 1.809 -4.077
1.809 29.321 -5.435
-4.077 -5.435 29.228

orbtensor 24 H
-15.413 -1.328 -3.297
-1.328 5.956 -1.732
-3.297 -1.732 9.920
28.573 -3.447 3.839
-3.447 29.908 -7.020
3.839 -7.020 23.308

orbtensor 25 H
-8.310 7.027 -8.198
7.027 -4.500 4.538
-8.198 4.538 -6.744
30.891 -7.813 7.529
-7.813 28.312 -0.939
7.529 -0.939 32.016

orbtensor 26 H
-1.028 -3.416 -3.005
-3.416 4.378 -4.492
-3.005 -4.492 7.519
25.904 -0.336 -1.210
-0.336 26.443 3.174
-1.210 3.174 32.191

orbtensor 27 H
-4.115 5.928 -6.499
5.928 -1.051 2.813
-6.499 2.813 0.760
30.019 -6.297 5.336
-6.297 25.865 -2.062
5.336 -2.062 30.004

orbtensor 28 H
-1.883 -1.926 4.558

-1.926	4.227	-0.402
4.558	-0.402	-0.290
32.977	-0.142	-4.845
-0.142	24.849	1.708
-4.845	1.708	24.992

orbtensor 29 H

-6.004	0.007	7.224
0.007	1.640	-1.694
7.224	-1.694	0.939
33.151	0.110	-4.445
0.110	25.391	-1.021
-4.445	-1.021	26.085

orbtensor 30 H

0.575	-0.676	3.733
-0.676	-1.548	-1.993
3.733	-1.993	-5.072
23.465	1.909	-8.236
1.909	29.690	5.195
-8.236	5.195	34.683

orbtensor 31 H

-4.912	6.631	-0.922
6.631	-0.246	-0.824
-0.922	-0.824	5.928
31.417	-7.666	1.661
-7.666	28.939	0.413
1.661	0.413	23.241

orbtensor 32 H

0.393	-5.065	1.478
-5.065	-5.275	0.813
1.478	0.813	0.072
25.247	11.024	-2.907
11.024	36.789	0.387
-2.907	0.387	24.485

orbtensor 33 H

-9.103	0.206	4.588
0.206	3.422	-0.093
4.588	-0.093	0.719
34.126	-2.846	-1.991
-2.846	24.231	0.603
-1.991	0.603	26.254

orbtensor 34 H

-1.827	-1.817	-3.584
-1.817	3.272	-0.946
-3.584	-0.946	2.597
27.429	2.813	5.003
2.813	29.229	2.158
5.003	2.158	27.223

orbtensor 35 H

-4.984	1.079	0.194
1.079	2.360	-1.049
0.194	-1.049	5.549
33.038	-2.260	-3.941
-2.260	24.597	-0.916
-3.941	-0.916	24.516

orbtensor 36 H

-6.181	-4.614	2.965
-4.614	4.146	0.503
2.965	0.503	5.038
34.512	6.266	-0.978

6.266 25.660 -2.085
 -0.978 -2.085 23.338

orbtensor 37 H
 -8.084 3.745 3.575
 3.745 1.771 -4.487
 3.575 -4.487 2.146
 31.201 -1.693 -4.762
 -1.693 25.724 2.553
 -4.762 2.553 27.531

orbtensor 38 H
 -4.678 1.374 -5.169
 1.374 4.571 -0.244
 -5.169 -0.244 1.908
 32.085 0.430 5.584
 0.430 21.919 -0.946
 5.584 -0.946 28.507

orbtensor 39 H
 -2.308 2.346 -3.982
 2.346 -1.886 4.455
 -3.982 4.455 -1.183
 28.544 -3.404 7.732
 -3.404 28.930 -10.326
 7.732 -10.326 28.912

gtensor (ppt)
 -0.196 -0.004 0.012
 -0.004 -0.187 0.004
 0.012 0.004 -0.204
 63.517 -10.832 -13.092
 -10.832 31.241 -17.121
 -13.092 -17.121 55.545

averaging
 NH2 Average:3,8,30,32,39

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.7673	29.18033	-166.73495	3.02459	-163.71037	-134.53003
3	H	0.0633	27.31900	-13.76179	0.43519	-13.32660	13.99240
4	H	0.1467	23.78433	-31.86941	-0.13854	-32.00795	-8.22362
5	H	0.0453	28.16467	-9.85054	-2.72193	-12.57247	15.59219
6	H	0.0527	29.64233	-11.44401	4.25299	-7.19103	22.45130
7	H	0.0843	29.93500	-18.32491	1.61410	-16.71081	13.22419
8	H	0.0050	27.57600	-1.08646	0.52715	-0.55931	27.01669
9	H	0.1890	26.40233	-41.06808	-2.72569	-43.79376	-17.39143
10	H	0.0827	30.72567	-17.96276	6.61518	-11.34757	19.37809
11	H	0.1087	24.82400	-23.61233	2.04302	-21.56932	3.25468
12	H	0.0210	28.22567	-4.56312	-0.68704	-5.25016	22.97550
13	H	-0.0187	29.82433	4.05611	1.55556	5.61166	35.43600
14	H	0.0517	25.15333	-11.22672	-7.35784	-18.58457	6.56877
15	H	-0.1563	28.39667	33.96989	-1.89221	32.07768	60.47435
16	H	-0.1423	24.07067	30.92781	0.51139	31.43921	55.50987
17	H	0.6627	28.19233	-143.99178	-1.55871	-145.55049	-117.35815
18	H	0.4237	29.05267	-92.05913	1.13012	-90.92901	-61.87634
19	H	0.9603	28.10800	-208.67220	0.72311	-207.94909	-179.84109
20	H	-0.0277	23.71467	6.01173	-0.30604	5.70569	29.42035
21	H	0.0787	28.92800	-17.09359	-0.48617	-17.57977	11.34823
22	H	0.0683	24.27067	-14.84825	0.83875	-14.00950	10.26117
23	H	0.3983	27.64033	-86.55442	-2.40127	-88.95569	-61.31536
24	H	0.0163	27.41733	-3.54909	-2.09539	-5.64449	21.77285

25	H	0.2203	23.88833	-47.87654	0.13937	-47.73717	-23.84884
26	H	0.0133	31.80233	-2.89722	5.12665	2.22943	34.03176
27	H	1.1197	27.16067	-243.29396	-1.18042	-244.47439	-217.31372
28	H	-0.0617	28.29067	13.39964	-1.88326	11.51637	39.80704
29	H	0.1233	27.06733	-26.79928	-2.25230	-29.05157	-1.98424
30	H	0.0030	27.26433	-0.65187	-0.33120	-0.98307	26.28126
31	H	0.3997	28.12233	-86.84414	-0.95098	-87.79512	-59.67279
32	H	0.0663	27.23700	-14.41366	0.17789	-14.23577	13.00123
33	H	0.1353	26.54967	-29.40677	-3.58637	-32.99314	-6.44348
34	H	-0.1167	29.30767	25.35067	0.02303	25.37369	54.68136
35	H	0.0470	28.35867	-10.21270	-1.28719	-11.49989	16.85878
36	H	0.8437	28.83767	-183.32153	-0.03290	-183.35443	-154.51676
37	H	0.1413	26.76300	-30.71052	-2.92905	-33.63957	-6.87657
38	H	0.3667	28.10400	-79.67352	-0.73626	-80.40979	-52.30579
39	H	0.0490	27.00300	-10.64728	-0.28472	-10.93200	16.07100
NH2 Average		0.0373	27.27987	-8.11221	0.10486	-8.00735	19.27252

=====
FeL4-STO-PBE0-No-G
Temperature: 298
Spin: 2

atensor 2 H
-0.333 0.253 0.258
0.253 0.931 1.741
0.258 1.741 1.746
-0.040 -0.008 -0.010
0.006 -0.013 0.016
0.015 0.046 0.011

atensor 3 H
-0.203 -0.036 -0.038
-0.036 0.031 0.369
-0.038 0.369 0.368
-0.008 -0.003 -0.005
0.001 -0.004 0.003
0.001 0.011 0.006

atensor 4 H
-0.411 -0.035 0.022
-0.035 0.853 -0.743
0.022 -0.743 -0.004
-0.019 0.000 0.005
0.003 0.018 -0.011
0.004 -0.027 0.003

atensor 5 H
-2.267 0.017 -0.316
0.017 -2.011 -1.069
-0.316 -1.069 4.379
-0.072 0.024 -0.037
0.019 -0.027 -0.052
0.003 -0.011 0.134

atensor 6 H
-1.059 0.891 2.479
0.891 -1.660 1.954
2.479 1.954 2.945
-0.068 0.025 0.044
0.000 -0.050 -0.006
0.073 0.067 0.050

atensor 7 H
-0.659 -0.770 -0.423
-0.770 1.213 1.155
-0.423 1.155 -0.277

-0.016 -0.038 -0.018
-0.004 0.011 0.024
-0.002 0.030 -0.019

atensor 8 H
-0.336 -0.185 -0.220
-0.185 0.093 0.576
-0.220 0.576 0.265
-0.008 -0.010 -0.011
0.000 -0.003 0.007
-0.002 0.017 0.004

atensor 9 H
-1.670 -1.361 1.348
-1.361 1.009 -3.441
1.348 -3.441 1.197
-0.067 -0.029 0.061
-0.021 0.050 -0.071
0.064 -0.092 0.048

atensor 10 H
-1.780 1.915 0.094
1.915 4.427 0.588
0.094 0.588 -2.300
-0.073 0.045 0.020
0.042 0.053 0.031
0.001 -0.038 -0.079

atensor 11 H
-0.294 0.442 0.235
0.442 0.747 0.660
0.235 0.660 -0.098
-0.017 0.006 0.006
0.007 0.003 0.011
0.006 0.009 -0.015

atensor 12 H
0.196 -3.900 -2.083
-3.900 1.498 2.504
-2.083 2.504 -1.627
0.046 -0.143 -0.075
-0.042 0.018 0.075
-0.035 0.084 -0.068

atensor 13 H
-1.455 -2.259 0.206
-2.259 3.715 -0.461
0.206 -0.461 -2.290
-0.040 -0.096 0.024
-0.029 0.076 0.011
0.037 -0.030 -0.062

atensor 14 H
0.434 1.339 -4.329
1.339 -2.573 -1.550
-4.329 -1.550 2.190
0.036 0.058 -0.137
0.052 -0.035 -0.025
-0.132 -0.029 0.103

atensor 15 H
-0.622 0.695 -0.975
0.695 -0.379 -1.183
-0.975 -1.183 0.504
-0.011 0.030 -0.031
0.021 0.003 -0.018
-0.029 -0.035 0.036

atensor 16 H
-0.452 0.111 0.246
0.111 -0.437 0.296
0.246 0.296 0.468
-0.011 0.002 0.002
0.001 -0.007 -0.002
0.008 0.009 0.012

atensor 17 H
-0.046 -0.118 -1.217
-0.118 -0.417 0.344
-1.217 0.344 2.428
-0.011 -0.001 -0.052
0.012 -0.019 -0.001
-0.027 0.019 0.053

atensor 18 H
-0.205 -1.115 -0.719
-1.115 1.306 1.409
-0.719 1.409 0.184
-0.009 -0.051 -0.030
-0.006 0.007 0.029
-0.009 0.041 -0.012

atensor 19 H
0.344 1.195 -0.469
1.195 2.454 -1.010
-0.469 -1.010 0.093
-0.024 0.040 -0.005
0.029 0.024 -0.006
-0.021 -0.049 -0.010

atensor 20 H
-0.218 -0.288 0.227
-0.288 0.164 -0.425
0.227 -0.425 -0.034
-0.006 -0.008 0.009
-0.005 0.008 -0.008
0.010 -0.012 0.003

atensor 21 H
0.030 -0.864 -0.965
-0.864 -0.014 0.950
-0.965 0.950 0.213
0.010 -0.031 -0.037
-0.004 -0.005 0.018
-0.021 0.033 0.002

atensor 22 H
-0.068 0.408 0.015
0.408 0.512 0.067
0.015 0.067 -0.228
-0.006 0.011 0.004
0.007 0.005 0.004
-0.002 -0.005 -0.010

atensor 23 H
0.161 0.880 -1.394
0.880 -0.066 -1.165
-1.394 -1.165 1.066
0.000 0.039 -0.043
0.026 -0.003 -0.016
-0.045 -0.034 0.037

atensor 24 H
5.479 0.492 1.608

0.492 -2.833 0.050
1.608 0.050 -2.614
0.165 0.035 0.060
-0.033 -0.061 0.021
0.000 0.036 -0.087

atensor 25 H
-0.003 -0.051 0.712
-0.051 -0.352 -0.049
0.712 -0.049 1.016
-0.011 0.003 0.018
-0.005 -0.008 -0.012
0.022 0.002 0.019

atensor 26 H
1.699 3.021 1.885
3.021 -0.190 1.365
1.885 1.365 -1.389
0.026 0.090 0.067
0.024 -0.031 0.026
0.015 0.020 -0.075

atensor 27 H
1.328 -0.979 1.472
-0.979 0.502 -0.999
1.472 -0.999 1.514
0.002 -0.021 0.053
-0.027 0.005 -0.028
0.046 -0.016 0.008

atensor 28 H
0.608 0.716 -1.152
0.716 -0.658 -0.519
-1.152 -0.519 -0.162
0.025 0.028 -0.033
0.018 -0.008 -0.002
-0.043 -0.013 0.010

atensor 29 H
1.010 -1.402 -1.663
-1.402 -0.541 1.013
-1.663 1.013 -0.131
0.046 -0.048 -0.060
-0.010 -0.010 0.028
-0.045 0.043 -0.004

atensor 30 H
0.036 0.466 -0.347
0.466 0.092 -0.352
-0.347 -0.352 -0.125
0.002 0.017 -0.008
0.010 0.002 -0.003
-0.014 -0.014 0.002

atensor 31 H
0.947 -1.749 0.041
-1.749 0.990 0.004
0.041 0.004 -0.755
0.029 -0.060 0.008
-0.030 0.020 0.010
0.012 0.004 -0.032

atensor 32 H
0.052 0.369 -0.118
0.369 0.306 -0.170
-0.118 -0.170 -0.157
-0.001 0.012 -0.002

0.007 0.003 0.000
-0.007 -0.009 -0.004

atensor 33 H
1.577 0.412 -2.043
0.412 -1.274 -0.268
-2.043 -0.268 0.052
0.059 0.024 -0.064
0.016 -0.022 0.007
-0.069 0.000 0.014

atensor 34 H
1.134 0.041 1.231
0.041 -1.078 0.021
1.231 0.021 -0.405
0.033 0.007 0.041
-0.017 -0.018 -0.004
0.026 0.010 -0.016

atensor 35 H
1.621 -0.550 0.398
-0.550 -0.724 -0.094
0.398 -0.094 -0.775
0.052 -0.013 0.017
-0.022 -0.009 0.005
0.007 0.009 -0.024

atensor 36 H
2.514 1.404 -0.086
1.404 0.340 -0.094
-0.086 -0.094 -0.324
0.047 0.048 0.004
0.014 -0.015 0.009
-0.028 -0.006 -0.031

atensor 37 H
2.906 -0.696 -0.482
-0.696 -1.235 0.046
-0.482 0.046 -1.287
0.098 -0.016 -0.006
-0.027 -0.018 0.019
-0.022 0.020 -0.040

atensor 38 H
2.390 -0.133 1.172
-0.133 -0.851 -0.081
1.172 -0.081 -0.452
0.060 0.002 0.045
-0.026 -0.018 -0.001
0.022 0.010 -0.029

atensor 39 H
0.153 -0.262 0.298
-0.262 -0.031 -0.216
0.298 -0.216 0.021
0.003 -0.007 0.011
-0.008 0.002 -0.005
0.010 -0.004 -0.001

orbtensor 2 H
5.100 1.082 2.357
1.082 1.744 -5.557
2.357 -5.557 -5.206
23.913 2.081 -1.833
2.081 28.612 6.894
-1.833 6.894 33.378

orbtensor 3 H
2.118 0.992 -1.373
0.992 -0.390 -4.019
-1.373 -4.019 -6.219
21.852 -2.703 3.743
-2.703 24.816 8.062
3.743 8.062 39.780

orbtensor 4 H
-5.509 -8.239 1.951
-8.239 -12.710 5.688
1.951 5.688 -1.744
31.812 6.537 0.259
6.537 35.033 -7.075
0.259 -7.075 24.471

orbtensor 5 H
5.006 -1.573 0.204
-1.573 5.027 4.167
0.204 4.167 -10.005
29.627 -3.651 2.024
-3.651 27.931 -1.938
2.024 -1.938 26.908

orbtensor 6 H
6.762 -0.082 -6.481
-0.082 1.964 1.222
-6.481 1.222 -5.325
28.247 -2.677 3.535
-2.677 30.650 -3.257
3.535 -3.257 26.629

orbtensor 7 H
2.852 2.691 0.046
2.691 -1.457 -1.733
0.046 -1.733 5.258
22.375 -1.387 0.948
-1.387 34.002 -0.666
0.948 -0.666 26.775

orbtensor 8 H
-3.536 4.082 -1.578
4.082 -1.202 -0.803
-1.578 -0.803 -0.381
32.923 -9.570 4.657
-9.570 27.301 2.714
4.657 2.714 27.623

orbtensor 9 H
6.825 -0.228 -5.917
-0.228 -9.622 6.020
-5.917 6.020 -3.474
27.072 5.122 0.108
5.122 31.573 -0.339
0.108 -0.339 26.833

orbtensor 10 H
7.383 -3.886 -3.258
-3.886 -3.199 -1.203
-3.258 -1.203 2.336
24.098 -0.787 1.139
-0.787 27.510 2.592
1.139 2.592 34.049

orbtensor 11 H
1.234 -0.298 1.104
-0.298 -5.493 -8.687

1.104	-8.687	-12.573
22.737	3.167	-2.937
3.167	32.030	7.321
-2.937	7.321	36.537

orbtensor 12 H

-3.471	10.395	3.944
10.395	-1.179	-7.435
3.944	-7.435	7.421
23.184	-3.177	2.236
-3.177	23.306	4.420
2.236	4.420	35.416

orbtensor 13 H

4.763	4.424	-0.374
4.424	-6.194	1.643
-0.374	1.643	6.549
29.427	3.755	-1.165
3.755	29.637	-1.087
-1.165	-1.087	25.291

orbtensor 14 H

-0.887	-6.021	13.156
-6.021	4.010	1.358
13.156	1.358	-10.018
25.854	7.787	-2.365
7.787	31.803	1.871
-2.365	1.871	24.698

orbtensor 15 H

4.436	-1.398	2.680
-1.398	1.892	2.467
2.680	2.467	-4.135
23.733	1.704	1.884
1.704	26.267	-2.724
1.884	-2.724	32.997

orbtensor 16 H

-2.088	-1.454	-6.186
-1.454	-1.300	-4.171
-6.186	-4.171	-15.781
26.344	-1.879	6.836
-1.879	26.320	5.223
6.836	5.223	38.717

orbtensor 17 H

2.265	0.555	6.400
0.555	4.027	-2.246
6.400	-2.246	-5.230
24.073	-0.713	-5.916
-0.713	24.687	2.740
-5.916	2.740	34.755

orbtensor 18 H

2.993	1.653	1.521
1.653	-1.319	-5.255
1.521	-5.255	2.841
24.962	-1.701	-0.240
-1.701	32.297	6.201
-0.240	6.201	25.384

orbtensor 19 H

-0.915	-6.997	2.811
-6.997	-2.630	4.030
2.811	4.030	1.998
29.619	5.041	-1.415
5.041	32.986	-5.109

-1.415 -5.109 23.266

orbtensor 20 H

-1.618 3.759 -3.814
3.759 -11.187 8.901
-3.814 8.901 -7.430
28.575 -1.727 4.319
-1.727 34.014 -9.889
4.319 -9.889 28.790

orbtensor 21 H

-0.810 3.092 3.653
3.092 2.825 -1.578
3.653 -1.578 2.040
32.727 -2.461 -3.814
-2.461 22.632 1.425
-3.814 1.425 27.370

orbtensor 22 H

-2.012 -6.329 -0.786
-6.329 -16.093 -2.402
-0.786 -2.402 -0.503
24.390 7.354 -1.556
7.354 39.498 2.945
-1.556 2.945 27.532

orbtensor 23 H

2.701 -3.203 4.420
-3.203 -0.306 4.517
4.420 4.517 -2.020
23.997 1.809 -4.077
1.809 29.321 -5.435
-4.077 -5.435 29.228

orbtensor 24 H

-15.413 -1.328 -3.297
-1.328 5.956 -1.732
-3.297 -1.732 9.920
28.573 -3.447 3.839
-3.447 29.908 -7.020
3.839 -7.020 23.308

orbtensor 25 H

-8.310 7.027 -8.198
7.027 -4.500 4.538
-8.198 4.538 -6.744
30.891 -7.813 7.529
-7.813 28.312 -0.939
7.529 -0.939 32.016

orbtensor 26 H

-1.028 -3.416 -3.005
-3.416 4.378 -4.492
-3.005 -4.492 7.519
25.904 -0.336 -1.210
-0.336 26.443 3.174
-1.210 3.174 32.191

orbtensor 27 H

-4.115 5.928 -6.499
5.928 -1.051 2.813
-6.499 2.813 0.760
30.019 -6.297 5.336
-6.297 25.865 -2.062
5.336 -2.062 30.004

orbtensor 28 H

-1.883	-1.926	4.558
-1.926	4.227	-0.402
4.558	-0.402	-0.290
32.977	-0.142	-4.845
-0.142	24.849	1.708
-4.845	1.708	24.992

orbtensor 29 H

-6.004	0.007	7.224
0.007	1.640	-1.694
7.224	-1.694	0.939
33.151	0.110	-4.445
0.110	25.391	-1.021
-4.445	-1.021	26.085

orbtensor 30 H

0.575	-0.676	3.733
-0.676	-1.548	-1.993
3.733	-1.993	-5.072
23.465	1.909	-8.236
1.909	29.690	5.195
-8.236	5.195	34.683

orbtensor 31 H

-4.912	6.631	-0.922
6.631	-0.246	-0.824
-0.922	-0.824	5.928
31.417	-7.666	1.661
-7.666	28.939	0.413
1.661	0.413	23.241

orbtensor 32 H

0.393	-5.065	1.478
-5.065	-5.275	0.813
1.478	0.813	0.072
25.247	11.024	-2.907
11.024	36.789	0.387
-2.907	0.387	24.485

orbtensor 33 H

-9.103	0.206	4.588
0.206	3.422	-0.093
4.588	-0.093	0.719
34.126	-2.846	-1.991
-2.846	24.231	0.603
-1.991	0.603	26.254

orbtensor 34 H

-1.827	-1.817	-3.584
-1.817	3.272	-0.946
-3.584	-0.946	2.597
27.429	2.813	5.003
2.813	29.229	2.158
5.003	2.158	27.223

orbtensor 35 H

-4.984	1.079	0.194
1.079	2.360	-1.049
0.194	-1.049	5.549
33.038	-2.260	-3.941
-2.260	24.597	-0.916
-3.941	-0.916	24.516

orbtensor 36 H

-6.181	-4.614	2.965
-4.614	4.146	0.503
2.965	0.503	5.038

```

34.512    6.266   -0.978
6.266    25.660   -2.085
-0.978   -2.085    23.338

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orbtensor 37 H
-8.084    3.745    3.575
3.745    1.771   -4.487
3.575   -4.487    2.146
31.201   -1.693   -4.762
-1.693   25.724    2.553
-4.762    2.553    27.531

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orbtensor 38 H
-4.678    1.374   -5.169
1.374    4.571   -0.244
-5.169   -0.244    1.908
32.085    0.430    5.584
0.430   21.919   -0.946
5.584   -0.946    28.507

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orbtensor 39 H
-2.308    2.346   -3.982
2.346   -1.886    4.455
-3.982    4.455   -1.183
28.544   -3.404    7.732
-3.404   28.930  -10.326
7.732  -10.326    28.912

```

```

gtensor (ppt)
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000

```

averaging
NH2 Average:3,8,30,32,39

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.7673	29.18033	-162.68035	0.00000	-162.68035	-133.50001
3	H	0.0633	27.31900	-13.42714	0.00000	-13.42714	13.89186
4	H	0.1467	23.78433	-31.09442	0.00000	-31.09442	-7.31009
5	H	0.0453	28.16467	-9.61100	-0.00000	-9.61100	18.55366
6	H	0.0527	29.64233	-11.16572	0.00000	-11.16572	18.47661
7	H	0.0843	29.93500	-17.87929	0.00000	-17.87929	12.05571
8	H	0.0050	27.57600	-1.06004	-0.00000	-1.06004	26.51596
9	H	0.1890	26.40233	-40.06940	0.00000	-40.06940	-13.66707
10	H	0.0827	30.72567	-17.52595	-0.00000	-17.52595	13.19972
11	H	0.1087	24.82400	-23.03814	-0.00000	-23.03814	1.78586
12	H	0.0210	28.22567	-4.45216	0.00000	-4.45216	23.77351
13	H	-0.0187	29.82433	3.95747	0.00000	3.95747	33.78180
14	H	0.0517	25.15333	-10.95372	-0.00000	-10.95372	14.19962
15	H	-0.1563	28.39667	33.14382	0.00000	33.14382	61.54049
16	H	-0.1423	24.07067	30.17572	-0.00000	30.17572	54.24639
17	H	0.6627	28.19233	-140.49024	-0.00000	-140.49024	-112.29790
18	H	0.4237	29.05267	-89.82047	-0.00000	-89.82047	-60.76780
19	H	0.9603	28.10800	-203.59777	-0.00000	-203.59777	-175.48977
20	H	-0.0277	23.71467	5.86554	0.00000	5.86554	29.58020
21	H	0.0787	28.92800	-16.67792	-0.00000	-16.67792	12.25008
22	H	0.0683	24.27067	-14.48717	0.00000	-14.48717	9.78349
23	H	0.3983	27.64033	-84.44961	0.00000	-84.44961	-56.80928

24	H	0.0163	27.41733	-3.46279	0.00000	-3.46279	23.95455
25	H	0.2203	23.88833	-46.71230	0.00000	-46.71230	-22.82396
26	H	0.0133	31.80233	-2.82677	0.00000	-2.82677	28.97557
27	H	1.1197	27.16067	-237.37762	0.00000	-237.37762	-210.21695
28	H	-0.0617	28.29067	13.07379	0.00000	13.07379	41.36446
29	H	0.1233	27.06733	-26.14758	0.00000	-26.14758	0.91975
30	H	0.0030	27.26433	-0.63602	0.00000	-0.63602	26.62831
31	H	0.3997	28.12233	-84.73229	0.00000	-84.73229	-56.60996
32	H	0.0663	27.23700	-14.06316	-0.00000	-14.06316	13.17384
33	H	0.1353	26.54967	-28.69167	0.00000	-28.69167	-2.14200
34	H	-0.1167	29.30767	24.73420	-0.00000	24.73420	54.04186
35	H	0.0470	28.35867	-9.96435	-0.00000	-9.96435	18.39432
36	H	0.8437	28.83767	-178.86358	0.00000	-178.86358	-150.02591
37	H	0.1413	26.76300	-29.96371	0.00000	-29.96371	-3.20071
38	H	0.3667	28.10400	-77.73605	-0.00000	-77.73605	-49.63205
39	H	0.0490	27.00300	-10.38836	-0.00000	-10.38836	16.61464
NH2 Average		0.0373	27.27987	-7.91494	-0.00000	-7.91494	19.36492

=====
FeL4-STO-PBE0-No-PSOSO
Temperature: 298
Spin: 2

atensor 2 H
-0.333 0.253 0.258
0.253 0.931 1.741
0.258 1.741 1.746
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 H
-0.203 -0.036 -0.038
-0.036 0.031 0.369
-0.038 0.369 0.368
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 H
-0.411 -0.035 0.022
-0.035 0.853 -0.743
0.022 -0.743 -0.004
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 H
-2.267 0.017 -0.316
0.017 -2.011 -1.069
-0.316 -1.069 4.379
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H
-1.059 0.891 2.479
0.891 -1.660 1.954
2.479 1.954 2.945
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 H
-0.659 -0.770 -0.423
-0.770 1.213 1.155

-0.423 1.155 -0.277
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-0.336 -0.185 -0.220
-0.185 0.093 0.576
-0.220 0.576 0.265
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 H
-1.670 -1.361 1.348
-1.361 1.009 -3.441
1.348 -3.441 1.197
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-1.780 1.915 0.094
1.915 4.427 0.588
0.094 0.588 -2.300
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 H
-0.294 0.442 0.235
0.442 0.747 0.660
0.235 0.660 -0.098
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
0.196 -3.900 -2.083
-3.900 1.498 2.504
-2.083 2.504 -1.627
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 H
-1.455 -2.259 0.206
-2.259 3.715 -0.461
0.206 -0.461 -2.290
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
0.434 1.339 -4.329
1.339 -2.573 -1.550
-4.329 -1.550 2.190
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 H
-0.622 0.695 -0.975
0.695 -0.379 -1.183
-0.975 -1.183 0.504
0.000 0.000 0.000
0.000 0.000 0.000

0.000 0.000 0.000

atensor 16 H
-0.452 0.111 0.246
0.111 -0.437 0.296
0.246 0.296 0.468
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 H
-0.046 -0.118 -1.217
-0.118 -0.417 0.344
-1.217 0.344 2.428
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 H
-0.205 -1.115 -0.719
-1.115 1.306 1.409
-0.719 1.409 0.184
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 H
0.344 1.195 -0.469
1.195 2.454 -1.010
-0.469 -1.010 0.093
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 H
-0.218 -0.288 0.227
-0.288 0.164 -0.425
0.227 -0.425 -0.034
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H
0.030 -0.864 -0.965
-0.864 -0.014 0.950
-0.965 0.950 0.213
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 22 H
-0.068 0.408 0.015
0.408 0.512 0.067
0.015 0.067 -0.228
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 H
0.161 0.880 -1.394
0.880 -0.066 -1.165
-1.394 -1.165 1.066
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 H

5.479 0.492 1.608
0.492 -2.833 0.050
1.608 0.050 -2.614
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 H
-0.003 -0.051 0.712
-0.051 -0.352 -0.049
0.712 -0.049 1.016
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 H
1.699 3.021 1.885
3.021 -0.190 1.365
1.885 1.365 -1.389
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 H
1.328 -0.979 1.472
-0.979 0.502 -0.999
1.472 -0.999 1.514
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 H
0.608 0.716 -1.152
0.716 -0.658 -0.519
-1.152 -0.519 -0.162
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 29 H
1.010 -1.402 -1.663
-1.402 -0.541 1.013
-1.663 1.013 -0.131
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 H
0.036 0.466 -0.347
0.466 0.092 -0.352
-0.347 -0.352 -0.125
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 31 H
0.947 -1.749 0.041
-1.749 0.990 0.004
0.041 0.004 -0.755
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 32 H
0.052 0.369 -0.118
0.369 0.306 -0.170
-0.118 -0.170 -0.157

0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 33 H
1.577 0.412 -2.043
0.412 -1.274 -0.268
-2.043 -0.268 0.052
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 34 H
1.134 0.041 1.231
0.041 -1.078 0.021
1.231 0.021 -0.405
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 35 H
1.621 -0.550 0.398
-0.550 -0.724 -0.094
0.398 -0.094 -0.775
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 36 H
2.514 1.404 -0.086
1.404 0.340 -0.094
-0.086 -0.094 -0.324
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 37 H
2.906 -0.696 -0.482
-0.696 -1.235 0.046
-0.482 0.046 -1.287
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 H
2.390 -0.133 1.172
-0.133 -0.851 -0.081
1.172 -0.081 -0.452
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 39 H
0.153 -0.262 0.298
-0.262 -0.031 -0.216
0.298 -0.216 0.021
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 2 H
5.100 1.082 2.357
1.082 1.744 -5.557
2.357 -5.557 -5.206
23.913 2.081 -1.833
2.081 28.612 6.894
-1.833 6.894 33.378

orbtensor 3 H
2.118 0.992 -1.373
0.992 -0.390 -4.019
-1.373 -4.019 -6.219
21.852 -2.703 3.743
-2.703 24.816 8.062
3.743 8.062 39.780

orbtensor 4 H
-5.509 -8.239 1.951
-8.239 -12.710 5.688
1.951 5.688 -1.744
31.812 6.537 0.259
6.537 35.033 -7.075
0.259 -7.075 24.471

orbtensor 5 H
5.006 -1.573 0.204
-1.573 5.027 4.167
0.204 4.167 -10.005
29.627 -3.651 2.024
-3.651 27.931 -1.938
2.024 -1.938 26.908

orbtensor 6 H
6.762 -0.082 -6.481
-0.082 1.964 1.222
-6.481 1.222 -5.325
28.247 -2.677 3.535
-2.677 30.650 -3.257
3.535 -3.257 26.629

orbtensor 7 H
2.852 2.691 0.046
2.691 -1.457 -1.733
0.046 -1.733 5.258
22.375 -1.387 0.948
-1.387 34.002 -0.666
0.948 -0.666 26.775

orbtensor 8 H
-3.536 4.082 -1.578
4.082 -1.202 -0.803
-1.578 -0.803 -0.381
32.923 -9.570 4.657
-9.570 27.301 2.714
4.657 2.714 27.623

orbtensor 9 H
6.825 -0.228 -5.917
-0.228 -9.622 6.020
-5.917 6.020 -3.474
27.072 5.122 0.108
5.122 31.573 -0.339
0.108 -0.339 26.833

orbtensor 10 H
7.383 -3.886 -3.258
-3.886 -3.199 -1.203
-3.258 -1.203 2.336
24.098 -0.787 1.139
-0.787 27.510 2.592
1.139 2.592 34.049

orbtensor 11 H
1.234 -0.298 1.104

-0.298	-5.493	-8.687
1.104	-8.687	-12.573
22.737	3.167	-2.937
3.167	32.030	7.321
-2.937	7.321	36.537

orbtensor 12 H

-3.471	10.395	3.944
10.395	-1.179	-7.435
3.944	-7.435	7.421
23.184	-3.177	2.236
-3.177	23.306	4.420
2.236	4.420	35.416

orbtensor 13 H

4.763	4.424	-0.374
4.424	-6.194	1.643
-0.374	1.643	6.549
29.427	3.755	-1.165
3.755	29.637	-1.087
-1.165	-1.087	25.291

orbtensor 14 H

-0.887	-6.021	13.156
-6.021	4.010	1.358
13.156	1.358	-10.018
25.854	7.787	-2.365
7.787	31.803	1.871
-2.365	1.871	24.698

orbtensor 15 H

4.436	-1.398	2.680
-1.398	1.892	2.467
2.680	2.467	-4.135
23.733	1.704	1.884
1.704	26.267	-2.724
1.884	-2.724	32.997

orbtensor 16 H

-2.088	-1.454	-6.186
-1.454	-1.300	-4.171
-6.186	-4.171	-15.781
26.344	-1.879	6.836
-1.879	26.320	5.223
6.836	5.223	38.717

orbtensor 17 H

2.265	0.555	6.400
0.555	4.027	-2.246
6.400	-2.246	-5.230
24.073	-0.713	-5.916
-0.713	24.687	2.740
-5.916	2.740	34.755

orbtensor 18 H

2.993	1.653	1.521
1.653	-1.319	-5.255
1.521	-5.255	2.841
24.962	-1.701	-0.240
-1.701	32.297	6.201
-0.240	6.201	25.384

orbtensor 19 H

-0.915	-6.997	2.811
-6.997	-2.630	4.030
2.811	4.030	1.998
29.619	5.041	-1.415

5.041	32.986	-5.109
-1.415	-5.109	23.266

orbtensor 20 H

-1.618	3.759	-3.814
3.759	-11.187	8.901
-3.814	8.901	-7.430
28.575	-1.727	4.319
-1.727	34.014	-9.889
4.319	-9.889	28.790

orbtensor 21 H

-0.810	3.092	3.653
3.092	2.825	-1.578
3.653	-1.578	2.040
32.727	-2.461	-3.814
-2.461	22.632	1.425
-3.814	1.425	27.370

orbtensor 22 H

-2.012	-6.329	-0.786
-6.329	-16.093	-2.402
-0.786	-2.402	-0.503
24.390	7.354	-1.556
7.354	39.498	2.945
-1.556	2.945	27.532

orbtensor 23 H

2.701	-3.203	4.420
-3.203	-0.306	4.517
4.420	4.517	-2.020
23.997	1.809	-4.077
1.809	29.321	-5.435
-4.077	-5.435	29.228

orbtensor 24 H

-15.413	-1.328	-3.297
-1.328	5.956	-1.732
-3.297	-1.732	9.920
28.573	-3.447	3.839
-3.447	29.908	-7.020
3.839	-7.020	23.308

orbtensor 25 H

-8.310	7.027	-8.198
7.027	-4.500	4.538
-8.198	4.538	-6.744
30.891	-7.813	7.529
-7.813	28.312	-0.939
7.529	-0.939	32.016

orbtensor 26 H

-1.028	-3.416	-3.005
-3.416	4.378	-4.492
-3.005	-4.492	7.519
25.904	-0.336	-1.210
-0.336	26.443	3.174
-1.210	3.174	32.191

orbtensor 27 H

-4.115	5.928	-6.499
5.928	-1.051	2.813
-6.499	2.813	0.760
30.019	-6.297	5.336
-6.297	25.865	-2.062
5.336	-2.062	30.004

orbtensor 28 H
-1.883 -1.926 4.558
-1.926 4.227 -0.402
4.558 -0.402 -0.290
32.977 -0.142 -4.845
-0.142 24.849 1.708
-4.845 1.708 24.992

orbtensor 29 H
-6.004 0.007 7.224
0.007 1.640 -1.694
7.224 -1.694 0.939
33.151 0.110 -4.445
0.110 25.391 -1.021
-4.445 -1.021 26.085

orbtensor 30 H
0.575 -0.676 3.733
-0.676 -1.548 -1.993
3.733 -1.993 -5.072
23.465 1.909 -8.236
1.909 29.690 5.195
-8.236 5.195 34.683

orbtensor 31 H
-4.912 6.631 -0.922
6.631 -0.246 -0.824
-0.922 -0.824 5.928
31.417 -7.666 1.661
-7.666 28.939 0.413
1.661 0.413 23.241

orbtensor 32 H
0.393 -5.065 1.478
-5.065 -5.275 0.813
1.478 0.813 0.072
25.247 11.024 -2.907
11.024 36.789 0.387
-2.907 0.387 24.485

orbtensor 33 H
-9.103 0.206 4.588
0.206 3.422 -0.093
4.588 -0.093 0.719
34.126 -2.846 -1.991
-2.846 24.231 0.603
-1.991 0.603 26.254

orbtensor 34 H
-1.827 -1.817 -3.584
-1.817 3.272 -0.946
-3.584 -0.946 2.597
27.429 2.813 5.003
2.813 29.229 2.158
5.003 2.158 27.223

orbtensor 35 H
-4.984 1.079 0.194
1.079 2.360 -1.049
0.194 -1.049 5.549
33.038 -2.260 -3.941
-2.260 24.597 -0.916
-3.941 -0.916 24.516

orbtensor 36 H
-6.181 -4.614 2.965
-4.614 4.146 0.503

```

2.965    0.503    5.038
34.512   6.266   -0.978
6.266   25.660   -2.085
-0.978   -2.085   23.338

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orbtensor 37 H
-8.084   3.745    3.575
3.745    1.771   -4.487
3.575   -4.487    2.146
31.201   -1.693   -4.762
-1.693   25.724    2.553
-4.762    2.553   27.531

```

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orbtensor 38 H
-4.678   1.374   -5.169
1.374    4.571   -0.244
-5.169   -0.244    1.908
32.085    0.430    5.584
0.430   21.919   -0.946
5.584   -0.946   28.507

```

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orbtensor 39 H
-2.308    2.346   -3.982
2.346   -1.886    4.455
-3.982    4.455   -1.183
28.544   -3.404    7.732
-3.404   28.930  -10.326
7.732   -10.326   28.912

```

```

gtensor (ppt)
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000

```

averaging
NH2 Average:3,8,30,32,39

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.7813	29.18033	-165.64845	0.00000	-165.64845	-136.46812
3	H	0.0653	27.31900	-13.85115	0.00000	-13.85115	13.46785
4	H	0.1460	23.78433	-30.95308	0.00000	-30.95308	-7.16875
5	H	0.0337	28.16467	-7.13758	-0.00000	-7.13758	21.02708
6	H	0.0753	29.64233	-15.97122	0.00000	-15.97122	13.67111
7	H	0.0923	29.93500	-19.57535	-0.00000	-19.57535	10.35965
8	H	0.0073	27.57600	-1.55472	0.00000	-1.55472	26.02128
9	H	0.1787	26.40233	-37.87866	0.00000	-37.87866	-11.47632
10	H	0.1157	30.72567	-24.52219	0.00000	-24.52219	6.20348
11	H	0.1183	24.82400	-25.08754	-0.00000	-25.08754	-0.26354
12	H	0.0223	28.22567	-4.73483	0.00000	-4.73483	23.49083
13	H	-0.0100	29.82433	2.12007	-0.00000	2.12007	31.94441
14	H	0.0170	25.15333	-3.60413	-0.00000	-3.60413	21.54921
15	H	-0.1657	28.39667	35.12256	0.00000	35.12256	63.51923
16	H	-0.1403	24.07067	29.75171	0.00000	29.75171	53.82237
17	H	0.6550	28.19233	-138.86485	-0.00000	-138.86485	-110.67251
18	H	0.4283	29.05267	-90.80984	-0.00000	-90.80984	-61.75717
19	H	0.9637	28.10800	-204.30446	-0.00000	-204.30446	-176.19646
20	H	-0.0293	23.71467	6.21888	0.00000	6.21888	29.93355
21	H	0.0763	28.92800	-16.18323	-0.00000	-16.18323	12.74477
22	H	0.0720	24.27067	-15.26453	-0.00000	-15.26453	9.00613

23	H	0.3870	27.64033	-82.04686	0.00000	-82.04686	-54.40653
24	H	0.0107	27.41733	-2.26141	0.00000	-2.26141	25.15592
25	H	0.2203	23.88833	-46.71230	0.00000	-46.71230	-22.82396
26	H	0.0400	31.80233	-8.48030	0.00000	-8.48030	23.32204
27	H	1.1147	27.16067	-236.31758	0.00000	-236.31758	-209.15692
28	H	-0.0707	28.29067	14.98186	0.00000	14.98186	43.27252
29	H	0.1127	27.06733	-23.88617	0.00000	-23.88617	3.18117
30	H	0.0010	27.26433	-0.21201	0.00000	-0.21201	27.05233
31	H	0.3940	28.12233	-83.53092	0.00000	-83.53092	-55.40858
32	H	0.0670	27.23700	-14.20450	-0.00000	-14.20450	13.03250
33	H	0.1183	26.54967	-25.08754	-0.00000	-25.08754	1.46212
34	H	-0.1163	29.30767	24.66353	0.00000	24.66353	53.97119
35	H	0.0407	28.35867	-8.62163	-0.00000	-8.62163	19.73703
36	H	0.8433	28.83767	-178.79291	-0.00000	-178.79291	-149.95524
37	H	0.1280	26.76300	-27.13695	0.00000	-27.13695	-0.37395
38	H	0.3623	28.10400	-76.81735	-0.00000	-76.81735	-48.71335
39	H	0.0477	27.00300	-10.10569	0.00000	-10.10569	16.89731
NH2 Average		0.0377	27.27987	-7.98561	-0.00000	-7.98561	19.29425

=====

FeL4-STO-PBE0-No-ZORA

Temperature: 298

Spin: 2

atensor 2 H

-0.300 0.254 0.259
0.254 0.963 1.740
0.259 1.740 1.779
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 H

-0.201 -0.036 -0.038
-0.036 0.032 0.369
-0.038 0.369 0.371
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 4 H

-0.407 -0.034 0.022
-0.034 0.857 -0.743
0.022 -0.743 -0.001
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 H

-2.265 0.016 -0.315
0.016 -2.005 -1.069
-0.315 -1.069 4.374
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 6 H

-1.054 0.890 2.478
0.890 -1.658 1.952
2.478 1.952 2.944
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 H

-0.664 -0.770 -0.422

-0.770 1.205 1.154
-0.422 1.154 -0.282
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 8 H
-0.335 -0.185 -0.220
-0.185 0.093 0.576
-0.220 0.576 0.264
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 H
-1.671 -1.356 1.344
-1.356 1.003 -3.437
1.344 -3.437 1.195
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 10 H
-1.777 1.910 0.093
1.910 4.423 0.590
0.093 0.590 -2.296
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 H
-0.288 0.444 0.235
0.444 0.753 0.659
0.235 0.659 -0.092
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 12 H
0.198 -3.893 -2.080
-3.893 1.491 2.498
-2.080 2.498 -1.619
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 H
-1.451 -2.255 0.208
-2.255 3.714 -0.461
0.208 -0.461 -2.287
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 14 H
0.437 1.337 -4.318
1.337 -2.565 -1.542
-4.318 -1.542 2.187
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 H
-0.614 0.695 -0.974
0.694 -0.372 -1.181
-0.974 -1.181 0.512
0.000 0.000 0.000

0.000 0.000 0.000
0.000 0.000 0.000

atensor 16 H
-0.448 0.110 0.246
0.110 -0.433 0.296
0.246 0.296 0.470
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 H
-0.012 -0.118 -1.217
-0.118 -0.382 0.343
-1.217 0.343 2.463
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 18 H
-0.186 -1.115 -0.718
-1.115 1.326 1.409
-0.718 1.409 0.201
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 H
0.385 1.194 -0.468
1.194 2.497 -1.009
-0.468 -1.009 0.134
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 20 H
-0.220 -0.289 0.227
-0.289 0.162 -0.425
0.227 -0.425 -0.035
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 21 H
0.029 -0.863 -0.964
-0.863 -0.017 0.948
-0.964 0.948 0.210
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 22 H
-0.076 0.409 0.016
0.409 0.508 0.068
0.016 0.068 -0.239
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 23 H
0.180 0.879 -1.393
0.879 -0.046 -1.165
-1.393 -1.165 1.088
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 24 H
5.471 0.488 1.601
0.488 -2.828 0.048
1.601 0.048 -2.615
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 25 H
-0.001 -0.052 0.712
-0.052 -0.351 -0.050
0.712 -0.050 1.017
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 26 H
1.696 3.018 1.884
3.018 -0.187 1.364
1.884 1.364 -1.380
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 27 H
1.353 -0.979 1.471
-0.979 0.527 -0.999
1.471 -0.999 1.542
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 28 H
0.613 0.715 -1.151
0.715 -0.652 -0.517
-1.151 -0.517 -0.155
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 29 H
1.017 -1.402 -1.662
-1.402 -0.536 1.013
-1.662 1.013 -0.128
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 30 H
0.037 0.467 -0.348
0.467 0.092 -0.353
-0.348 -0.353 -0.124
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 31 H
0.985 -1.750 0.042
-1.750 1.030 0.004
0.042 0.004 -0.715
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 32 H
0.053 0.369 -0.118
0.369 0.307 -0.170

-0.118 -0.170 -0.154
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 33 H
1.581 0.411 -2.043
0.411 -1.268 -0.267
-2.043 -0.267 0.057
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 34 H
1.135 0.041 1.230
0.041 -1.074 0.021
1.230 0.021 -0.404
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 35 H
1.617 -0.550 0.396
-0.550 -0.726 -0.094
0.396 -0.094 -0.779
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 36 H
2.559 1.405 -0.085
1.405 0.385 -0.095
-0.085 -0.095 -0.279
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 37 H
2.910 -0.695 -0.482
-0.695 -1.230 0.046
-0.482 0.046 -1.283
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 38 H
2.406 -0.131 1.172
-0.131 -0.834 -0.081
1.172 -0.081 -0.435
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 39 H
0.155 -0.262 0.298
-0.262 -0.028 -0.216
0.298 -0.216 0.023
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 2 H
5.140 1.068 2.363
1.068 1.762 -5.589
2.363 -5.589 -5.222
23.918 2.080 -1.836
2.080 28.617 6.896

-1.836 6.896 33.389

orbtensor 3 H

2.122 0.984 -1.363
0.984 -0.394 -4.026
-1.363 -4.026 -6.219
21.863 -2.704 3.744
-2.704 24.828 8.065
3.744 8.065 39.797

orbtensor 4 H

-5.487 -8.239 1.955
-8.239 -12.733 5.704
1.955 5.704 -1.748
31.821 6.541 0.258
6.541 35.043 -7.076
0.258 -7.076 24.477

orbtensor 5 H

5.092 -1.584 0.186
-1.584 5.056 4.208
0.186 4.208 -10.152
29.638 -3.654 2.027
-3.654 27.942 -1.938
2.027 -1.938 26.912

orbtensor 6 H

6.785 -0.109 -6.564
-0.109 2.021 1.196
-6.564 1.196 -5.406
28.261 -2.682 3.533
-2.682 30.667 -3.264
3.533 -3.264 26.639

orbtensor 7 H

2.877 2.713 0.067
2.713 -1.475 -1.756
0.067 -1.756 5.283
22.377 -1.388 0.949
-1.388 34.012 -0.669
0.949 -0.669 26.781

orbtensor 8 H

-3.519 4.085 -1.564
4.085 -1.204 -0.818
-1.564 -0.818 -0.379
32.937 -9.574 4.658
-9.574 27.313 2.716
4.658 2.716 27.635

orbtensor 9 H

6.872 -0.185 -5.976
-0.185 -9.687 6.126
-5.976 6.126 -3.538
27.086 5.127 0.107
5.127 31.587 -0.335
0.107 -0.335 26.841

orbtensor 10 H

7.475 -3.925 -3.233
-3.925 -3.267 -1.228
-3.233 -1.228 2.398
24.110 -0.790 1.141
-0.790 27.515 2.597
1.141 2.597 34.069

orbtensor 11 H

1.248	-0.303	1.101
-0.303	-5.492	-8.704
1.101	-8.704	-12.567
22.743	3.166	-2.938
3.166	32.037	7.324
-2.938	7.324	36.550

orbtensor 12 H

-3.504	10.503	4.008
10.503	-1.224	-7.478
4.008	-7.478	7.481
23.201	-3.169	2.244
-3.169	23.316	4.412
2.244	4.412	35.443

orbtensor 13 H

4.789	4.489	-0.385
4.489	-6.310	1.680
-0.385	1.680	6.614
29.440	3.761	-1.165
3.761	29.645	-1.090
-1.165	-1.090	25.304

orbtensor 14 H

-0.862	-6.083	13.287
-6.083	4.060	1.362
13.287	1.362	-10.050
25.864	7.789	-2.357
7.789	31.823	1.879
-2.357	1.879	24.704

orbtensor 15 H

4.468	-1.423	2.710
-1.423	1.902	2.488
2.710	2.488	-4.156
23.735	1.705	1.886
1.705	26.270	-2.724
1.886	-2.724	33.008

orbtensor 16 H

-2.076	-1.465	-6.190
-1.465	-1.290	-4.176
-6.190	-4.176	-15.800
26.350	-1.879	6.839
-1.879	26.325	5.225
6.839	5.225	38.729

orbtensor 17 H

2.298	0.544	6.444
0.544	4.051	-2.256
6.444	-2.256	-5.267
24.078	-0.712	-5.920
-0.712	24.692	2.742
-5.920	2.742	34.768

orbtensor 18 H

3.009	1.679	1.549
1.679	-1.331	-5.285
1.549	-5.285	2.869
24.968	-1.703	-0.241
-1.703	32.306	6.205
-0.241	6.205	25.390

orbtensor 19 H

-0.880	-7.021	2.833
-7.021	-2.648	4.052
2.833	4.052	2.019

29.627	5.045	-1.416
5.045	32.993	-5.111
-1.416	-5.111	23.269

orbtensor 20 H

-1.613	3.776	-3.824
3.776	-11.199	8.912
-3.824	8.912	-7.440
28.581	-1.729	4.321
-1.729	34.024	-9.893
4.321	-9.893	28.798

orbtensor 21 H

-0.808	3.113	3.683
3.113	2.828	-1.603
3.683	-1.603	2.055
32.737	-2.462	-3.815
-2.462	22.635	1.427
-3.815	1.427	27.376

orbtensor 22 H

-2.010	-6.340	-0.787
-6.340	-16.102	-2.401
-0.787	-2.401	-0.487
24.394	7.357	-1.557
7.357	39.510	2.946
-1.557	2.946	27.537

orbtensor 23 H

2.731	-3.233	4.462
-3.233	-0.296	4.537
4.462	4.537	-2.045
24.001	1.812	-4.080
1.812	29.329	-5.437
-4.080	-5.437	29.235

orbtensor 24 H

-15.616	-1.319	-3.350
-1.319	5.985	-1.734
-3.350	-1.734	9.981
28.576	-3.449	3.835
-3.449	29.939	-7.024
3.835	-7.024	23.330

orbtensor 25 H

-8.310	7.025	-8.223
7.025	-4.490	4.550
-8.223	4.550	-6.767
30.901	-7.816	7.531
-7.816	28.321	-0.940
7.531	-0.940	32.024

orbtensor 26 H

-1.062	-3.496	-3.045
-3.496	4.418	-4.544
-3.045	-4.544	7.543
25.907	-0.340	-1.211
-0.340	26.455	3.176
-1.211	3.176	32.206

orbtensor 27 H

-4.145	5.965	-6.559
5.965	-1.055	2.847
-6.559	2.847	0.734
30.028	-6.301	5.339
-6.301	25.871	-2.063
5.339	-2.063	30.009

orbtensor 28 H
-1.889 -1.947 4.593
-1.947 4.244 -0.401
4.593 -0.401 -0.287
32.986 -0.142 -4.849
-0.142 24.855 1.711
-4.849 1.711 24.998

orbtensor 29 H
-6.051 0.042 7.287
0.042 1.649 -1.730
7.287 -1.730 0.966
33.158 0.111 -4.448
0.111 25.396 -1.022
-4.448 -1.022 26.090

orbtensor 30 H
0.580 -0.691 3.746
-0.691 -1.544 -1.983
3.746 -1.983 -5.073
23.475 1.910 -8.239
1.910 29.702 5.196
-8.239 5.196 34.698

orbtensor 31 H
-4.957 6.690 -0.934
6.690 -0.271 -0.822
-0.934 -0.822 5.965
31.425 -7.671 1.662
-7.671 28.948 0.413
1.662 0.413 23.247

orbtensor 32 H
0.388 -5.067 1.482
-5.067 -5.276 0.821
1.482 0.821 0.073
25.260 11.028 -2.909
11.028 36.805 0.386
-2.909 0.386 24.496

orbtensor 33 H
-9.156 0.187 4.661
0.187 3.452 -0.106
4.661 -0.106 0.730
34.135 -2.847 -1.991
-2.847 24.235 0.603
-1.991 0.603 26.258

orbtensor 34 H
-1.882 -1.813 -3.627
-1.813 3.288 -0.948
-3.627 -0.948 2.606
27.433 2.816 5.007
2.816 29.239 2.160
5.007 2.160 27.227

orbtensor 35 H
-5.049 1.096 0.177
1.096 2.370 -1.049
0.177 -1.049 5.569
33.048 -2.260 -3.944
-2.260 24.602 -0.918
-3.944 -0.918 24.522

orbtensor 36 H
-6.229 -4.648 2.976

```

-4.648    4.176    0.498
2.976     0.498    5.074
34.523    6.271    -0.977
6.271    25.668    -2.086
-0.977    -2.086    23.341

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orbtensor 37 H
-8.211    3.776    3.586
3.776     1.790   -4.503
3.586    -4.503    2.198
31.209   -1.694   -4.764
-1.694    25.730    2.554
-4.764    2.554    27.537

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orbtensor 38 H
-4.766    1.383   -5.216
1.383     4.595   -0.244
-5.216   -0.244    1.925
32.095    0.430    5.587
0.430    21.922   -0.948
5.587    -0.948    28.513

```

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orbtensor 39 H
-2.322    2.357   -3.990
2.357   -1.889    4.450
-3.990    4.450   -1.192
28.558   -3.405    7.736
-3.405    28.943  -10.329
7.736   -10.329    28.926

```

```

gtensor (ppt)
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000
0.000    0.000    0.000

```

averaging
NH2 Average:3,8,30,32,39

Final results. Shifts and Shieldings in ppm.

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.8140	29.20133	-172.57402	0.00000	-172.57402	-143.37269
3	H	0.0673	27.33233	-14.27516	0.00000	-14.27516	13.05717
4	H	0.1497	23.79100	-31.73044	-0.00000	-31.73044	-7.93944
5	H	0.0347	28.16267	-7.34959	0.00000	-7.34959	20.81308
6	H	0.0773	29.65567	-16.39524	0.00000	-16.39524	13.26043
7	H	0.0863	29.95167	-18.30331	0.00000	-18.30331	11.64836
8	H	0.0073	27.59433	-1.55472	0.00000	-1.55472	26.03961
9	H	0.1757	26.38700	-37.24263	0.00000	-37.24263	-10.85563
10	H	0.1167	30.76667	-24.73420	0.00000	-24.73420	6.03247
11	H	0.1243	24.83967	-26.35959	-0.00000	-26.35959	-1.51992
12	H	0.0233	28.23767	-4.94684	0.00000	-4.94684	23.29083
13	H	-0.0080	29.82733	1.69606	0.00000	1.69606	31.52339
14	H	0.0197	25.17967	-4.16948	0.00000	-4.16948	21.01019
15	H	-0.1580	28.40900	33.49717	-0.00000	33.49717	61.90617
16	H	-0.1370	24.07933	29.04501	0.00000	29.04501	53.12435
17	H	0.6897	28.20667	-146.21444	0.00000	-146.21444	-118.00777
18	H	0.4470	29.07033	-94.76731	0.00000	-94.76731	-65.69697
19	H	1.0053	28.12667	-213.13811	-0.00000	-213.13811	-185.01144
20	H	-0.0310	23.71700	6.57223	0.00000	6.57223	30.28923
21	H	0.0740	28.94100	-15.68855	-0.00000	-15.68855	13.25245

22	H	0.0643	24.28067	-13.63914	0.00000	-13.63914	10.64152
23	H	0.4073	27.65167	-86.35768	-0.00000	-86.35768	-58.70601
24	H	0.0093	27.39833	-1.97874	0.00000	-1.97874	25.41960
25	H	0.2217	23.89300	-46.99497	0.00000	-46.99497	-23.10197
26	H	0.0430	31.82233	-9.11632	-0.00000	-9.11632	22.70602
27	H	1.1407	27.14733	-241.82977	-0.00000	-241.82977	-214.68244
28	H	-0.0647	28.30233	13.70981	-0.00000	13.70981	42.01215
29	H	0.1177	27.06933	-24.94620	0.00000	-24.94620	2.12313
30	H	0.0017	27.27933	-0.35335	0.00000	-0.35335	26.92599
31	H	0.4333	28.11900	-91.86987	0.00000	-91.86987	-63.75087
32	H	0.0687	27.24867	-14.55784	0.00000	-14.55784	12.69083
33	H	0.1233	26.55133	-26.14758	-0.00000	-26.14758	0.40375
34	H	-0.1143	29.30367	24.23951	0.00000	24.23951	53.54318
35	H	0.0373	28.35400	-7.91494	-0.00000	-7.91494	20.43906
36	H	0.8883	28.85100	-188.33324	-0.00000	-188.33324	-159.48224
37	H	0.1323	26.75100	-28.05565	0.00000	-28.05565	-1.30465
38	H	0.3790	28.09467	-80.35080	0.00000	-80.35080	-52.25614
39	H	0.0500	27.00800	-10.60037	-0.00000	-10.60037	16.40763
NH2 Average		0.0390	27.29253	-8.26829	-0.00000	-8.26829	19.02424

=====
3NiCp2-STO-PBE0-acetonitrile

Temperature: 298

Spin: 1

atensor 1 Ni

122.494 0.000 0.005
0.000 122.496 0.006
0.005 0.006 17.095
-46.428 -0.001 -0.004
-0.001 -46.425 -0.003
-0.004 -0.003 -2.468

atensor 2 H

-6.649 -2.441 -1.069
-2.441 -0.650 3.006
-1.069 3.007 -3.302
-0.145 -0.071 -0.084
-0.071 0.029 0.236
-0.008 0.024 0.010

atensor 3 C

1.316 -0.323 -1.012
-0.323 2.109 2.847
-1.012 2.847 12.439
-0.304 -0.038 -0.070
-0.038 -0.211 0.196
-0.005 0.014 -0.010

atensor 4 H

0.212 0.212 -3.190
0.212 -7.510 -0.087
-3.190 -0.087 -3.302
0.054 0.006 -0.251
0.006 -0.170 -0.007
-0.025 -0.001 0.010

atensor 5 C

2.223 0.028 -3.021
0.028 1.202 -0.083
-3.021 -0.083 12.438
-0.197 0.003 -0.208
0.003 -0.318 -0.006
-0.015 0.000 -0.010

atensor 6 H
-6.896 2.098 -0.903
2.098 -0.399 -3.061
-0.903 -3.061 -3.301
-0.152 0.061 -0.071
0.061 0.036 -0.241
-0.007 -0.024 0.010

atensor 7 C
1.285 0.277 -0.855
0.277 2.144 -2.898
-0.855 -2.898 12.435
-0.308 0.033 -0.059
0.033 -0.207 -0.200
-0.004 -0.014 -0.010

atensor 8 H
-2.252 -3.606 2.632
-3.606 -5.041 -1.804
2.633 -1.805 -3.299
-0.017 -0.105 0.207
-0.104 -0.098 -0.142
0.021 -0.014 0.010

atensor 9 C
1.899 -0.477 2.492
-0.477 1.530 -1.708
2.492 -1.708 12.430
-0.236 -0.056 0.172
-0.056 -0.279 -0.118
0.012 -0.008 -0.010

atensor 10 H
-2.656 3.737 2.529
3.737 -4.639 1.946
2.529 1.946 -3.300
-0.029 0.108 0.199
0.108 -0.086 0.153
0.020 0.015 0.010

atensor 11 C
1.843 0.494 2.395
0.494 1.581 1.842
2.395 1.842 12.432
-0.242 0.058 0.165
0.058 -0.273 0.127
0.012 0.009 -0.010

atensor 12 H
-6.895 2.098 0.903
2.098 -0.401 3.062
0.903 3.062 -3.299
-0.152 0.061 0.071
0.061 0.036 0.241
0.007 0.024 0.010

atensor 13 C
1.284 0.278 0.855
0.278 2.142 2.896
0.855 2.896 12.430
-0.308 0.033 0.059
0.033 -0.207 0.200
0.004 0.014 -0.010

atensor 14 H
-2.256 -3.606 -2.632
-3.606 -5.045 1.804

-2.633 1.804 -3.301
-0.017 -0.104 -0.207
-0.104 -0.098 0.142
-0.021 0.014 0.010

atensor 15 C
1.895 -0.476 -2.491
-0.476 1.527 1.706
-2.491 1.706 12.438
-0.236 -0.056 -0.172
-0.056 -0.279 0.118
-0.012 0.008 -0.010

atensor 16 H
-2.660 3.738 -2.528
3.738 -4.642 -1.946
-2.529 -1.946 -3.303
-0.029 0.108 -0.199
0.108 -0.087 -0.153
-0.020 -0.015 0.010

atensor 17 C
1.840 0.494 -2.393
0.494 1.579 -1.843
-2.393 -1.843 12.440
-0.242 0.058 -0.165
0.058 -0.273 -0.127
-0.012 -0.009 -0.010

atensor 18 H
-6.648 -2.441 1.069
-2.441 -0.651 -3.007
1.069 -3.007 -3.302
-0.145 -0.071 0.084
-0.071 0.029 -0.236
0.008 -0.024 0.010

atensor 19 C
1.315 -0.323 1.012
-0.323 2.108 -2.847
1.012 -2.847 12.435
-0.305 -0.038 0.070
-0.038 -0.211 -0.196
0.005 -0.014 -0.010

atensor 20 C
2.224 0.028 3.020
0.028 1.203 0.082
3.020 0.082 12.427
-0.197 0.003 0.208
0.003 -0.318 0.006
0.015 0.000 -0.010

atensor 21 H
0.213 0.212 3.191
0.212 -7.507 0.087
3.191 0.087 -3.299
0.054 0.006 0.251
0.006 -0.170 0.007
0.025 0.001 0.010

orbtensor 1 Ni
-12032.455 -0.250 -0.482
-0.250-12031.673 -0.671
-0.482 -0.671 -373.877
2258.352 -0.001 0.002
-0.001 2258.354 -0.001

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0.002    -0.001  2270.626

orbtensor 2 H
-0.477    5.166    0.755
5.166   -13.171   -2.122
0.755    -2.122   -0.285
27.575   -5.007   -0.769
-5.007   39.876    2.162
-0.769    2.162   24.810

orbtensor 3 C
-178.237   14.366    6.766
14.366  -213.514  -19.029
6.766   -19.029  -64.609
256.662    2.688   -1.440
2.688   250.052    4.043
-1.440    4.043  233.036

orbtensor 4 H
-14.997   -0.447    2.250
-0.447    1.345    0.062
2.250     0.062   -0.285
41.645     0.434   -2.293
0.434   25.808   -0.063
-2.293   -0.063   24.810

orbtensor 5 C
-218.607   -1.247   20.185
-1.247  -173.182    0.550
20.185    0.550  -64.605
249.105   -0.233   -4.290
-0.233   257.614   -0.117
-4.290   -0.117  233.036

orbtensor 6 H
0.047   -4.439    0.637
-4.439  -13.699    2.158
0.637    2.158   -0.287
27.067    4.301   -0.649
4.301   40.388   -2.199
-0.649   -2.199   24.811

orbtensor 7 C
-176.782  -12.341    5.707
-12.341  -214.998   19.356
5.707   19.356  -64.608
256.937   -2.315   -1.215
-2.315  249.780   -4.113
-1.215   -4.113  233.034

orbtensor 8 H
-9.776    7.632   -1.857
7.632   -3.874    1.271
-1.857    1.271   -0.286
36.587   -7.395    1.891
-7.395   30.867   -1.296
1.891   -1.296   24.810

orbtensor 9 C
-204.078   21.218  -16.643
21.218  -187.682   11.411
-16.643   11.411  -64.610
251.817    3.974    3.539
3.974   254.895   -2.423
3.539   -2.423  233.034

orbtensor 10 H

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-8.922	-7.910	-1.785
-7.910	-4.727	-1.373
-1.785	-1.373	-0.285
35.758	7.666	1.819
7.666	31.693	1.400
1.819	1.400	24.810

orbtensor 11 C

-201.701	-21.991	-16.000
-21.991	-190.037	-12.312
-16.000	-12.312	-64.606
252.262	-4.118	3.400
-4.118	254.449	2.619
3.400	2.619	233.036

orbtensor 12 H

0.049	-4.441	-0.637
-4.441	-13.701	-2.157
-0.637	-2.157	-0.286
27.066	4.303	0.647
4.303	40.392	2.197
0.647	2.197	24.810

orbtensor 13 C

-176.748	-12.355	-5.704
-12.355	-215.034	-19.405
-5.704	-19.405	-64.621
256.941	-2.311	1.207
-2.311	249.793	4.106
1.207	4.106	233.044

orbtensor 14 H

-9.779	7.633	1.857
7.633	-3.875	-1.271
1.857	-1.271	-0.285
36.590	-7.397	-1.890
-7.397	30.868	1.295
-1.890	1.295	24.810

orbtensor 15 C

-204.144	21.245	16.696
21.245	-187.711	-11.447
16.696	-11.447	-64.624
251.834	3.969	-3.533
3.969	254.907	2.418
-3.533	2.418	233.042

orbtensor 16 H

-8.925	-7.912	1.783
-7.912	-4.728	1.372
1.783	1.372	-0.283
35.761	7.668	-1.816
7.668	31.694	-1.397
-1.816	-1.397	24.808

orbtensor 17 C

-201.772	-22.020	16.049
-22.020	-190.085	12.327
16.049	12.327	-64.613
252.279	-4.112	-3.396
-4.112	254.463	-2.608
-3.396	-2.608	233.043

orbtensor 18 H

-0.475	5.167	-0.753
5.167	-13.174	2.119
-0.753	2.119	-0.283

27.574 -5.008 0.766
 -5.008 39.880 -2.158
 0.766 -2.158 24.808

orbtensor 19 C
 -178.212 14.381 -6.760
 14.381 -213.573 19.052
 -6.760 19.052 -64.616
 256.666 2.685 1.430
 2.685 250.067 -4.034
 1.430 -4.034 233.042

orbtensor 20 C
 -218.635 -1.244 -20.202
 -1.244 -173.120 -0.559
 -20.202 -0.559 -64.616
 249.116 -0.234 4.280
 -0.234 257.613 0.118
 4.280 0.118 233.045

orbtensor 21 H
 -14.999 -0.447 -2.248
 -0.447 1.349 -0.061
 -2.248 -0.061 -0.284
 41.648 0.434 2.289
 0.434 25.806 0.063
 2.289 0.063 24.808

gtensor (ppt)
 -0.089 0.000 0.000
 0.000 -0.089 0.000
 0.000 0.000 -0.231
 91.357 0.004 0.008
 0.004 91.347 0.005
 0.008 0.005 0.815

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
 Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.5880	-5883.55767	45221.78081	488.14458	45709.92539	39826.36772
2	H	-3.5690	26.10933	259.90650	0.29594	260.20244	286.31177
3	C	5.1130	94.46333	-1480.48260	31.03194	-1449.45066	-1354.98732
4	H	-3.5687	26.10867	259.88222	0.29530	260.17752	286.28619
5	C	5.1127	94.45367	-1480.38608	31.03147	-1449.35461	-1354.90094
6	H	-3.5673	26.10900	259.78513	0.29553	260.08066	286.18966
7	C	5.1130	94.45433	-1480.48260	31.01741	-1449.46519	-1355.01086
8	H	-3.5657	26.10933	259.66375	0.29503	259.95879	286.06812
9	C	5.1113	94.45867	-1480.00001	31.00009	-1448.99993	-1354.54126
10	H	-3.5667	26.10900	259.73658	0.29393	260.03051	286.13951
11	C	5.1103	94.46767	-1479.71046	31.01079	-1448.69967	-1354.23201
12	H	-3.5670	26.11000	259.76085	0.29621	260.05706	286.16706
13	C	5.1103	94.45833	-1479.71046	31.00337	-1448.70709	-1354.24876
14	H	-3.5690	26.10967	259.90650	0.29705	260.20354	286.31321
15	C	5.1117	94.43467	-1480.09653	31.03482	-1449.06171	-1354.62705
16	H	-3.5703	26.10900	260.00360	0.29611	260.29971	286.40871
17	C	5.1113	94.43833	-1480.00001	31.04598	-1448.95403	-1354.51570
18	H	-3.5690	26.11000	259.90650	0.29626	260.20276	286.31276
19	C	5.1107	94.45800	-1479.80698	31.02607	-1448.78091	-1354.32291
20	C	5.1097	94.46767	-1479.51743	30.99277	-1448.52465	-1354.05699
21	H	-3.5663	26.10933	259.71230	0.29473	260.00704	286.11637

C Average	5.1114	94.45547	-1480.01932	31.01947	-1448.99985	-1354.54438
H Average	-3.5679	26.10933	259.82639	0.29561	260.12200	286.23134

=====
 3NiCp2-STO-PBE0-toluene
 Temperature: 298
 Spin: 1

atensor 1 Ni
 122.382 0.001 0.005
 0.001 122.382 0.006
 0.005 0.006 17.197
 -46.105 0.001 -0.004
 0.001 -46.103 -0.003
 -0.004 -0.003 -2.505

atensor 2 H
 -6.683 -2.452 -1.067
 -2.452 -0.658 3.002
 -1.068 3.002 -3.317
 -0.144 -0.070 -0.083
 -0.070 0.028 0.234
 -0.009 0.024 0.010

atensor 3 C
 1.142 -0.325 -1.005
 -0.325 1.940 2.826
 -1.005 2.826 12.396
 -0.304 -0.037 -0.069
 -0.037 -0.212 0.194
 -0.006 0.016 -0.010

atensor 4 H
 0.208 0.213 -3.185
 0.213 -7.548 -0.087
 -3.185 -0.087 -3.318
 0.052 0.006 -0.248
 0.006 -0.169 -0.007
 -0.026 -0.001 0.010

atensor 5 C
 2.055 0.028 -2.998
 0.028 1.027 -0.082
 -2.998 -0.082 12.396
 -0.199 0.003 -0.206
 0.003 -0.317 -0.006
 -0.017 0.000 -0.010

atensor 6 H
 -6.931 2.107 -0.901
 2.107 -0.407 -3.056
 -0.901 -3.057 -3.316
 -0.151 0.060 -0.070
 0.060 0.035 -0.238
 -0.007 -0.025 0.010

atensor 7 C
 1.110 0.279 -0.848
 0.279 1.975 -2.877
 -0.848 -2.877 12.392
 -0.307 0.032 -0.058
 0.032 -0.208 -0.198
 -0.005 -0.016 -0.010

atensor 8 H
 -2.268 -3.621 2.628

-3.621 -5.068 -1.802
2.629 -1.802 -3.315
-0.018 -0.104 0.205
-0.103 -0.098 -0.140
0.021 -0.015 0.010

atensor 9 C
1.727 -0.480 2.474
-0.480 1.356 -1.696
2.474 -1.696 12.387
-0.237 -0.055 0.170
-0.055 -0.279 -0.117
0.014 -0.009 -0.010

atensor 10 H
-2.673 3.753 2.525
3.753 -4.664 1.943
2.526 1.943 -3.315
-0.030 0.107 0.197
0.107 -0.087 0.151
0.020 0.016 0.010

atensor 11 C
1.672 0.497 2.377
0.497 1.408 1.829
2.377 1.829 12.389
-0.243 0.057 0.164
0.057 -0.273 0.126
0.013 0.010 -0.010

atensor 12 H
-6.930 2.107 0.901
2.107 -0.407 3.057
0.901 3.057 -3.314
-0.152 0.060 0.070
0.060 0.035 0.238
0.007 0.025 0.010

atensor 13 C
1.108 0.279 0.848
0.279 1.972 2.875
0.848 2.875 12.387
-0.308 0.032 0.058
0.032 -0.208 0.198
0.005 0.016 -0.010

atensor 14 H
-2.271 -3.622 -2.628
-3.622 -5.072 1.801
-2.628 1.801 -3.317
-0.018 -0.103 -0.205
-0.103 -0.098 0.140
-0.021 0.015 0.010

atensor 15 C
1.724 -0.480 -2.473
-0.480 1.353 1.694
-2.473 1.694 12.397
-0.237 -0.055 -0.170
-0.055 -0.279 0.117
-0.014 0.009 -0.010

atensor 16 H
-2.676 3.754 -2.524
3.754 -4.667 -1.942
-2.525 -1.943 -3.318
-0.030 0.107 -0.197

0.107 -0.087 -0.151
-0.020 -0.016 0.010

atensor 17 C
1.670 0.497 -2.376
0.497 1.407 -1.829
-2.376 -1.829 12.398
-0.243 0.057 -0.163
0.057 -0.273 -0.126
-0.013 -0.010 -0.010

atensor 18 H
-6.682 -2.452 1.067
-2.452 -0.658 -3.002
1.067 -3.002 -3.317
-0.144 -0.070 0.083
-0.070 0.028 -0.234
0.009 -0.024 0.010

atensor 19 C
1.141 -0.325 1.005
-0.325 1.939 -2.826
1.005 -2.826 12.393
-0.304 -0.037 0.069
-0.037 -0.212 -0.194
0.006 -0.016 -0.010

atensor 20 C
2.056 0.028 2.998
0.028 1.027 0.081
2.998 0.081 12.386
-0.199 0.003 0.206
0.003 -0.317 0.006
0.016 0.000 -0.010

atensor 21 H
0.209 0.213 3.185
0.213 -7.545 0.087
3.186 0.087 -3.315
0.053 0.006 0.248
0.006 -0.169 0.007
0.026 0.001 0.010

orbtensor 1 Ni
-11941.131 0.201 -0.446
0.201-11940.296 -0.637
-0.446 -0.637 -378.357
2258.499 0.000 0.002
0.000 2258.501 -0.001
0.002 -0.001 2270.667

orbtensor 2 H
-0.509 5.135 0.751
5.135 -13.126 -2.112
0.751 -2.112 -0.279
27.742 -4.969 -0.773
-4.969 39.951 2.176
-0.773 2.176 24.992

orbtensor 3 C
-177.083 14.676 6.865
14.676 -213.127 -19.293
6.865 -19.293 -64.956
256.519 2.583 -1.434
2.583 250.171 4.035
-1.434 4.035 232.985

orbtensor 4 H
-14.939 -0.446 2.241
-0.446 1.305 0.061
2.241 0.061 -0.279
41.705 0.432 -2.307
0.432 25.984 -0.063
-2.307 -0.063 24.989

orbtensor 5 C
-218.308 -1.276 20.465
-1.276 -171.909 0.561
20.465 0.561 -64.945
249.260 -0.224 -4.280
-0.224 257.433 -0.114
-4.280 -0.114 232.986

orbtensor 6 H
0.015 -4.413 0.634
-4.413 -13.650 2.149
0.634 2.149 -0.279
27.234 4.270 -0.653
4.270 40.459 -2.213
-0.653 -2.213 24.992

orbtensor 7 C
-175.570 -12.615 5.789
-12.615 -214.623 19.629
5.789 19.629 -64.954
256.782 -2.220 -1.215
-2.220 249.907 -4.105
-1.215 -4.105 232.985

orbtensor 8 H
-9.751 7.586 -1.849
7.586 -3.883 1.267
-1.849 1.267 -0.279
36.685 -7.341 1.903
-7.341 31.007 -1.305
1.903 -1.305 24.991

orbtensor 9 C
-203.462 21.683 -16.882
21.683 -186.702 11.568
-16.882 11.568 -64.955
251.866 3.817 3.530
3.817 254.820 -2.421
3.530 -2.421 232.986

orbtensor 10 H
-8.902 -7.862 -1.777
-7.862 -4.732 -1.366
-1.777 -1.366 -0.279
35.864 7.608 1.830
7.608 31.828 1.408
1.830 1.408 24.992

orbtensor 11 C
-201.044 -22.466 -16.222
-22.466 -189.140 -12.490
-16.222 -12.490 -64.954
252.293 -3.955 3.394
-3.955 254.393 2.611
3.394 2.611 232.986

orbtensor 12 H
0.018 -4.413 -0.634
-4.413 -13.648 -2.152

-0.634	-2.152	-0.279
27.233	4.271	0.653
4.271	40.458	2.216
0.653	2.216	24.992

orbtensor 13 C

-175.545	-12.613	-5.783
-12.613	-214.611	-19.664
-5.783	-19.664	-64.958
256.779	-2.219	1.206
-2.219	249.905	4.109
1.206	4.109	232.989

orbtensor 14 H

-9.750	7.586	1.852
7.586	-3.883	-1.269
1.852	-1.269	-0.279
36.685	-7.342	-1.907
-7.342	31.007	1.306
-1.907	1.306	24.992

orbtensor 15 C

-203.494	21.678	16.921
21.678	-186.725	-11.597
16.921	-11.597	-64.961
251.871	3.816	-3.535
3.816	254.823	2.419
-3.535	2.419	232.987

orbtensor 16 H

-8.902	-7.862	1.778
-7.862	-4.732	1.368
1.778	1.368	-0.279
35.864	7.609	-1.831
7.609	31.828	-1.408
-1.831	-1.408	24.991

orbtensor 17 C

-201.082	-22.462	16.258
-22.462	-189.170	12.490
16.258	12.490	-64.954
252.299	-3.954	-3.396
-3.954	254.398	-2.609
-3.396	-2.609	232.986

orbtensor 18 H

-0.508	5.135	-0.751
5.135	-13.126	2.112
-0.751	2.112	-0.279
27.740	-4.969	0.773
-4.969	39.952	-2.175
0.773	-2.175	24.991

orbtensor 19 C

-177.066	14.670	-6.850
14.670	-213.135	19.301
-6.850	19.301	-64.955
256.517	2.582	1.430
2.582	250.173	-4.034
1.430	-4.034	232.987

orbtensor 20 C

-218.285	-1.271	-20.469
-1.271	-171.858	-0.568
-20.469	-0.568	-64.950
249.256	-0.225	4.278
-0.225	257.426	0.118

4.278 0.118 232.988

orbtensor 21 H

-14.937 -0.446 -2.242
-0.446 1.308 -0.061
-2.242 -0.061 -0.279
41.704 0.431 2.308
0.431 25.982 0.063
2.308 0.063 24.989

gtensor (ppt)

-0.089 0.000 0.000
0.000 -0.089 0.000
0.000 0.000 -0.231
90.342 -0.002 0.007
-0.002 90.331 0.005
0.007 0.005 0.826

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.7493	-5824.03900	45338.22820	483.75375	45821.98194	39997.94294
2	H	-3.5880	26.25700	261.20488	0.29647	261.50135	287.75835
3	C	4.9840	94.83633	-1442.65938	31.04104	-1411.61834	-1316.78201
4	H	-3.5883	26.25500	261.22914	0.29573	261.52487	287.77987
5	C	4.9840	94.83900	-1442.65938	31.04335	-1411.61603	-1316.77703
6	H	-3.5867	26.25700	261.10781	0.29709	261.40490	287.66190
7	C	4.9840	94.84233	-1442.65938	31.02707	-1411.63231	-1316.78998
8	H	-3.5857	26.25667	261.03501	0.29543	261.33044	287.58711
9	C	4.9813	94.85100	-1441.88749	31.01394	-1410.87355	-1316.02255
10	H	-3.5863	26.25700	261.08354	0.29611	261.37965	287.63665
11	C	4.9810	94.84467	-1441.79100	31.02231	-1410.76869	-1315.92402
12	H	-3.5860	26.25800	261.05928	0.29744	261.35671	287.61471
13	C	4.9803	94.85300	-1441.59803	31.01753	-1410.58050	-1315.72750
14	H	-3.5887	26.25733	261.25341	0.29695	261.55036	287.80769
15	C	4.9827	94.83367	-1442.27343	31.05200	-1411.22143	-1316.38777
16	H	-3.5893	26.25667	261.30194	0.29745	261.59939	287.85606
17	C	4.9830	94.82567	-1442.36992	31.05667	-1411.31325	-1316.48758
18	H	-3.5877	26.25667	261.18061	0.29649	261.47710	287.73377
19	C	4.9823	94.84033	-1442.17695	31.03682	-1411.14013	-1316.29979
20	C	4.9810	94.85900	-1441.79100	31.00984	-1410.78116	-1315.92216
21	H	-3.5857	26.25567	261.03501	0.29496	261.32997	287.58564
	C Average	4.9824	94.84250	-1442.18660	31.03206	-1411.15454	-1316.31204
	H Average	-3.5872	26.25670	261.14906	0.29641	261.44547	287.70217

3NiCp2-STO-PBE0-water

Temperature: 298

Spin: 1

atensor 1 Ni

122.486 0.001 0.005
0.001 122.487 0.006
0.005 0.006 17.169
-46.259 0.001 -0.004
0.001 -46.260 -0.003
-0.004 -0.003 -2.481

atensor 2 H

-6.659 -2.443 -1.067
-2.443 -0.656 3.002
-1.067 3.002 -3.313
-0.144 -0.070 -0.084
-0.070 0.029 0.235
-0.009 0.024 0.010

atensor 3 C
1.297 -0.323 -1.013
-0.323 2.090 2.849
-1.013 2.849 12.444
-0.304 -0.038 -0.070
-0.038 -0.211 0.196
-0.005 0.014 -0.010

atensor 4 H
0.207 0.212 -3.184
0.212 -7.522 -0.087
-3.185 -0.087 -3.313
0.053 0.006 -0.249
0.006 -0.169 -0.007
-0.025 -0.001 0.010

atensor 5 C
2.203 0.028 -3.023
0.028 1.182 -0.083
-3.023 -0.083 12.443
-0.197 0.003 -0.208
0.003 -0.318 -0.006
-0.015 0.000 -0.010

atensor 6 H
-6.908 2.099 -0.901
2.099 -0.406 -3.056
-0.901 -3.056 -3.312
-0.151 0.060 -0.071
0.060 0.036 -0.239
-0.007 -0.024 0.010

atensor 7 C
1.264 0.277 -0.855
0.277 2.123 -2.901
-0.855 -2.901 12.440
-0.308 0.033 -0.059
0.033 -0.207 -0.199
-0.004 -0.014 -0.010

atensor 8 H
-2.260 -3.609 2.628
-3.609 -5.051 -1.802
2.628 -1.802 -3.311
-0.018 -0.104 0.206
-0.104 -0.098 -0.141
0.021 -0.014 0.010

atensor 9 C
1.878 -0.477 2.494
-0.477 1.509 -1.710
2.494 -1.710 12.435
-0.236 -0.056 0.171
-0.056 -0.279 -0.118
0.012 -0.009 -0.010

atensor 10 H
-2.663 3.740 2.525
3.740 -4.648 1.943
2.525 1.943 -3.311

-0.029 0.107 0.198
0.107 -0.086 0.152
0.020 0.015 0.010

atensor 11 C
1.824 0.494 2.397
0.494 1.562 1.844
2.397 1.844 12.437
-0.242 0.058 0.165
0.058 -0.273 0.127
0.012 0.009 -0.010

atensor 12 H
-6.907 2.099 0.901
2.099 -0.407 3.057
0.901 3.057 -3.311
-0.151 0.060 0.071
0.060 0.036 0.239
0.007 0.024 0.010

atensor 13 C
1.264 0.278 0.855
0.278 2.122 2.898
0.855 2.899 12.436
-0.309 0.033 0.059
0.033 -0.207 0.199
0.004 0.014 -0.010

atensor 14 H
-2.264 -3.609 -2.628
-3.609 -5.055 1.801
-2.628 1.801 -3.313
-0.018 -0.104 -0.206
-0.104 -0.098 0.141
-0.021 0.014 0.010

atensor 15 C
1.876 -0.477 -2.493
-0.476 1.507 1.708
-2.493 1.708 12.445
-0.236 -0.056 -0.171
-0.056 -0.280 0.117
-0.012 0.009 -0.010

atensor 16 H
-2.667 3.741 -2.524
3.741 -4.651 -1.942
-2.525 -1.943 -3.314
-0.029 0.107 -0.198
0.107 -0.086 -0.152
-0.020 -0.015 0.010

atensor 17 C
1.822 0.494 -2.395
0.494 1.561 -1.844
-2.395 -1.844 12.446
-0.242 0.058 -0.165
0.058 -0.273 -0.127
-0.012 -0.009 -0.010

atensor 18 H
-6.659 -2.443 1.067
-2.443 -0.656 -3.002
1.067 -3.002 -3.313
-0.144 -0.070 0.084
-0.070 0.029 -0.235
0.008 -0.024 0.010

atensor 19 C
1.297 -0.323 1.013
-0.323 2.090 -2.849
1.013 -2.849 12.441
-0.305 -0.038 0.070
-0.038 -0.211 -0.196
0.005 -0.014 -0.010

atensor 20 C
2.205 0.028 3.022
0.028 1.184 0.082
3.022 0.082 12.434
-0.197 0.003 0.208
0.003 -0.318 0.006
0.015 0.000 -0.010

atensor 21 H
0.207 0.212 3.186
0.212 -7.519 0.087
3.186 0.087 -3.311
0.053 0.006 0.250
0.006 -0.169 0.007
0.025 0.001 0.010

orbtensor 1 Ni
-11982.164 0.210 -0.459
0.210-11982.582 -0.690
-0.459 -0.690 -374.209
2258.433 0.000 0.002
0.000 2258.432 -0.001
0.002 -0.001 2270.703

orbtensor 2 H
-0.483 5.164 0.752
5.164 -13.170 -2.114
0.752 -2.114 -0.284
27.545 -5.019 -0.774
-5.019 39.876 2.176
-0.774 2.176 24.792

orbtensor 3 C
-178.459 14.328 6.750
14.328 -213.649 -18.989
6.750 -18.989 -64.615
256.682 2.690 -1.445
2.690 250.074 4.057
-1.445 4.057 233.073

orbtensor 4 H
-14.994 -0.449 2.243
-0.449 1.342 0.062
2.243 0.062 -0.283
41.649 0.436 -2.309
0.436 25.771 -0.064
-2.309 -0.064 24.791

orbtensor 5 C
-218.704 -1.242 20.143
-1.242 -173.380 0.546
20.143 0.546 -64.611
249.124 -0.235 -4.306
-0.235 257.631 -0.118
-4.306 -0.118 233.072

orbtensor 6 H
0.048 -4.438 0.634

-4.438	-13.697	2.153
0.634	2.153	-0.282
27.029	4.314	-0.654
4.314	40.388	-2.216
-0.654	-2.216	24.791

orbtensor 7 C

-176.940	-12.324	5.700
-12.324	-215.083	19.318
5.700	19.318	-64.610
256.952	-2.310	-1.220
-2.310	249.796	-4.131
-1.220	-4.131	233.073

orbtensor 8 H

-9.775	7.630	-1.851
7.630	-3.874	1.269
-1.851	1.269	-0.282
36.577	-7.416	1.906
-7.416	30.841	-1.306
1.906	-1.306	24.791

orbtensor 9 C

-204.194	21.177	-16.613
21.177	-187.812	11.383
-16.613	11.383	-64.613
251.836	3.973	3.553
3.973	254.909	-2.434
3.553	-2.434	233.073

orbtensor 10 H

-8.923	-7.907	-1.778
-7.907	-4.728	-1.368
-1.778	-1.368	-0.283
35.748	7.684	1.830
7.684	31.671	1.409
1.830	1.409	24.792

orbtensor 11 C

-201.848	-21.937	-15.965
-21.937	-190.222	-12.287
-15.965	-12.287	-64.613
252.282	-4.119	3.411
-4.119	254.466	2.628
3.411	2.628	233.072

orbtensor 12 H

0.050	-4.439	-0.634
-4.439	-13.699	-2.152
-0.634	-2.152	-0.281
27.028	4.315	0.652
4.315	40.392	2.214
0.652	2.214	24.790

orbtensor 13 C

-176.913	-12.334	-5.696
-12.334	-215.119	-19.368
-5.696	-19.368	-64.622
256.959	-2.307	1.211
-2.307	249.809	4.124
1.211	4.124	233.084

orbtensor 14 H

-9.778	7.632	1.850
7.632	-3.874	-1.269
1.850	-1.269	-0.281
36.579	-7.418	-1.904

-7.418	30.842	1.305
-1.904	1.305	24.790

orbtensor 15 C

-204.265	21.198	16.667
21.198	-187.850	-11.421
16.667	-11.421	-64.626
251.853	3.969	-3.546
3.969	254.924	2.428
-3.546	2.428	233.082

orbtensor 16 H

-8.925	-7.909	1.776
-7.909	-4.730	1.367
1.776	1.367	-0.282
35.751	7.687	-1.827
7.687	31.673	-1.406
-1.827	-1.406	24.790

orbtensor 17 C

-201.919	-21.965	16.015
-21.965	-190.269	12.302
16.015	12.302	-64.620
252.302	-4.113	-3.406
-4.113	254.481	-2.617
-3.406	-2.617	233.080

orbtensor 18 H

-0.481	5.166	-0.751
5.166	-13.174	2.111
-0.751	2.111	-0.282
27.544	-5.020	0.771
-5.020	39.880	-2.171
0.771	-2.171	24.790

orbtensor 19 C

-178.434	14.342	-6.744
14.342	-213.705	19.013
-6.744	19.013	-64.621
256.688	2.688	1.435
2.688	250.090	-4.047
1.435	-4.047	233.080

orbtensor 20 C

-218.727	-1.239	-20.162
-1.239	-173.317	-0.556
-20.162	-0.556	-64.621
249.136	-0.236	4.294
-0.236	257.632	0.119
4.294	0.119	233.082

orbtensor 21 H

-14.996	-0.449	-2.241
-0.449	1.346	-0.062
-2.241	-0.062	-0.281
41.652	0.436	2.304
0.436	25.769	0.064
2.304	0.064	24.790

gtensor (ppt)

90.801	-0.002	0.007
-0.002	90.806	0.006
0.007	0.006	0.815
-0.088	0.000	0.000
0.000	-0.088	0.000
0.000	0.000	-0.231

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	55.7140	-5850.46233	45316.26625	485.96722	45802.23347	39951.77114
2	H	-3.5777	26.09200	260.49155	0.29069	260.78223	286.87423
3	C	5.1020	94.36867	-1477.03619	30.91115	-1446.12505	-1351.75638
4	H	-3.5780	26.09200	260.51582	0.29240	260.80822	286.90022
5	C	5.1010	94.37733	-1476.74669	30.91453	-1445.83216	-1351.45483
6	H	-3.5770	26.09233	260.44301	0.29211	260.73511	286.82745
7	C	5.1007	94.39600	-1476.65019	30.90326	-1445.74693	-1351.35093
8	H	-3.5760	26.09267	260.37020	0.29132	260.66152	286.75418
9	C	5.0990	94.39967	-1476.16769	30.88624	-1445.28145	-1350.88178
10	H	-3.5757	26.09233	260.34592	0.29077	260.63669	286.72902
11	C	5.0993	94.37900	-1476.26419	30.89146	-1445.37274	-1350.99374
12	H	-3.5767	26.09333	260.41874	0.29160	260.71034	286.80367
13	C	5.0987	94.39933	-1476.07119	30.89029	-1445.18090	-1350.78156
14	H	-3.5793	26.09267	260.61290	0.29311	260.90600	286.99867
15	C	5.1007	94.37267	-1476.65019	30.92277	-1445.72742	-1351.35475
16	H	-3.5790	26.09233	260.58863	0.29256	260.88119	286.97352
17	C	5.1013	94.35167	-1476.84319	30.92637	-1445.91683	-1351.56516
18	H	-3.5777	26.09233	260.49155	0.29120	260.78275	286.87508
19	C	5.1007	94.36600	-1476.65019	30.90606	-1445.74413	-1351.37813
20	C	5.0993	94.39500	-1476.26419	30.87941	-1445.38478	-1350.98978
21	H	-3.5763	26.09333	260.39447	0.29164	260.68610	286.77943
	C Average	5.1003	94.38053	-1476.53439	30.90315	-1445.63124	-1351.25070
	H Average	-3.5773	26.09253	260.46728	0.29174	260.75901	286.85155

FeL3-STO-PBE0-acetontrile

Temperature: 298

Spin: 2

atensor 2 H

-0.211 -0.113 0.010
-0.113 1.661 -0.369
0.010 -0.369 -0.134
-0.014 -0.005 0.001
0.000 0.030 -0.006
0.001 -0.009 -0.002

atensor 3 H

-0.848 0.160 -0.103
0.160 0.958 -1.097
-0.103 -1.097 -0.131
-0.019 0.001 0.001
0.007 0.026 -0.024
-0.001 -0.014 0.005

atensor 20 H

0.304 -0.883 -0.920
-0.883 -0.298 0.681
-0.920 0.681 -0.125
0.016 -0.022 -0.027
-0.017 -0.003 0.019
-0.004 0.008 -0.002

atensor 23 H

0.617 0.657 1.012
0.657 -0.656 0.405

1.012 0.405 -0.177
0.015 0.018 0.024
0.006 -0.015 0.007
0.005 0.006 -0.007

atensor 24 H
1.033 0.900 0.268
0.900 0.297 0.177
0.268 0.177 -0.248
0.016 0.023 0.009
0.012 -0.007 0.006
-0.001 0.003 -0.008

atensor 25 H
1.311 -0.752 -0.327
-0.752 0.093 0.167
-0.328 0.167 -0.197
0.026 -0.017 -0.009
-0.021 -0.001 0.009
0.001 0.004 -0.005

orbtensor 2 H
4.084 4.148 2.541
4.148 -13.017 -3.435
2.541 -3.435 -0.360
19.055 -4.642 -2.857
-4.642 41.025 2.815
-2.857 2.815 24.352

orbtensor 3 H
3.716 0.553 4.586
0.553 -4.681 1.493
4.586 1.493 -8.452
19.686 0.038 -6.288
0.038 26.139 -4.033
-6.288 -4.033 38.450

orbtensor 20 H
-3.721 2.991 -1.319
2.991 2.235 -5.359
-1.319 -5.359 -7.560
24.564 -2.433 0.006
-2.433 21.321 7.816
0.006 7.816 38.191

orbtensor 23 H
-1.860 -3.350 -3.797
-3.350 0.723 3.749
-3.797 3.749 -6.838
24.805 2.474 7.280
2.474 21.752 -3.991
7.280 -3.991 37.665

orbtensor 24 H
-4.500 -9.173 1.344
-9.173 -4.056 4.113
1.344 4.113 0.447
30.558 11.842 -0.496
11.842 29.668 -3.986
-0.496 -3.986 23.937

orbtensor 25 H
-13.243 5.118 -4.188
5.118 3.859 -1.339
-4.188 -1.339 0.483
40.252 -6.443 3.265
-6.443 19.982 1.492

3.265 1.492 23.840

gtensor (ppt)

-0.191 0.009 0.000
0.009 -0.183 -0.001
0.000 -0.001 -0.167
53.305 -8.293 -3.584
-8.293 44.501 -9.257
-3.584 -9.257 17.884

averaging

Cis Average:3,20,23

Trans Average:2,24,25

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4433	25.04633	-95.79167	-0.64722	-96.43889	-71.39256
3	H	-0.0030	24.95267	0.64821	-0.50672	0.14150	25.09416
4	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
5	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
7	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
8	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
9	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
10	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
11	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
12	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
13	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
14	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
15	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
16	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
17	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
19	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
20	H	-0.0360	25.01000	7.77857	-0.50650	7.27207	32.28207
21	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	H	-0.0743	25.41567	16.06131	0.59756	16.65887	42.07454
24	H	0.3610	25.35133	-78.00179	-0.06893	-78.07071	-52.71938
25	H	0.4090	25.05767	-88.37321	-1.28305	-89.65626	-64.59859
26	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
27	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
28	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
29	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
30	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
31	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
32	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
33	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
34	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
35	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
36	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
37	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
38	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
39	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000

FeL3-STO-PBE0-water

Temperature: 298

Spin: 2

atensor 2 H

-0.212 -0.113 0.010

-0.113 1.661 -0.368

0.010 -0.368 -0.134
-0.014 -0.005 0.001
0.000 0.030 -0.007
0.001 -0.009 -0.002

atensor 3 H
-0.848 0.160 -0.103
0.160 0.958 -1.097
-0.103 -1.097 -0.131
-0.019 0.001 0.001
0.007 0.026 -0.024
-0.001 -0.014 0.005

atensor 20 H
0.304 -0.883 -0.920
-0.883 -0.298 0.681
-0.920 0.681 -0.125
0.016 -0.022 -0.027
-0.017 -0.003 0.019
-0.004 0.008 -0.002

atensor 23 H
0.618 0.657 1.012
0.657 -0.655 0.406
1.012 0.406 -0.177
0.015 0.018 0.024
0.007 -0.015 0.007
0.005 0.006 -0.007

atensor 24 H
1.034 0.900 0.269
0.900 0.297 0.177
0.269 0.177 -0.247
0.016 0.023 0.009
0.012 -0.007 0.006
-0.001 0.003 -0.008

atensor 25 H
1.311 -0.752 -0.328
-0.752 0.093 0.167
-0.328 0.167 -0.197
0.026 -0.017 -0.009
-0.021 -0.001 0.009
0.001 0.004 -0.005

orbtensor 2 H
3.239 4.052 2.352
4.052 -12.908 -3.383
2.352 -3.383 -0.431
19.051 -4.651 -2.862
-4.651 40.994 2.830
-2.862 2.830 24.336

orbtensor 3 H
3.449 0.646 4.454
0.646 -4.676 1.376
4.454 1.376 -8.431
19.718 0.034 -6.293
0.034 26.170 -4.030
-6.293 -4.030 38.461

orbtensor 20 H
-3.721 2.757 -1.332
2.757 2.018 -5.181
-1.332 -5.181 -7.443
24.580 -2.434 0.007
-2.434 21.331 7.813

0.007 7.813 38.198

orbtensor 23 H

-1.925 -3.196 -3.606
-3.196 0.807 3.663
-3.606 3.663 -6.839
24.826 2.476 7.274
2.476 21.773 -3.991
7.274 -3.991 37.676

orbtensor 24 H

-4.588 -8.802 1.596
-8.802 -4.650 3.971
1.596 3.971 0.324
30.540 11.836 -0.503
11.836 29.657 -3.993
-0.503 -3.993 23.929

orbtensor 25 H

-13.317 4.704 -4.038
4.704 2.996 -0.938
-4.038 -0.938 0.288
40.245 -6.439 3.270
-6.439 19.976 1.490
3.270 1.490 23.838

gtensor (ppt)

-0.191 0.009 0.000
0.009 -0.184 -0.001
0.000 -0.001 -0.167
51.138 -8.680 -2.766
-8.680 43.395 -9.312
-2.766 -9.312 17.714

averaging

Cis Average:3,20,23

Trans Average:2,24,25

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Fe	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
2	H	0.4430	24.76033	-95.66580	-0.65751	-96.32330	-71.56297
3	H	-0.0030	24.89700	0.64785	-0.52888	0.11897	25.01597
4	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
5	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
6	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
7	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
8	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
9	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
10	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
11	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
12	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
13	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
14	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
15	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
16	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
17	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
18	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
19	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
20	H	-0.0360	24.98767	7.77420	-0.45811	7.31608	32.30375
21	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
22	H	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
23	H	-0.0737	25.43933	15.90831	0.58848	16.49679	41.93612
24	H	0.3617	25.07067	-78.10187	-0.01232	-78.11419	-53.04352

25	H	0.4090	24.67533	-88.32350	-1.22947	-89.55297	-64.87763
26	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
27	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
28	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
29	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
30	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
31	N	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
32	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
33	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
34	O	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
35	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
36	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
37	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
38	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000
39	C	0.0000	0.00000	0.00000	0.00000	0.00000	0.00000

=====
3NiCp2-STO-PBE0-DZ-DZ

Temperature: 298

Spin: 1

atensor 1 Ni

96.286 0.017 0.002
0.017 96.224 0.010
0.002 0.010 0.571
-40.990 -0.003 -0.003
-0.003 -40.967 -0.003
-0.003 -0.003 -2.912

atensor 2 H

-8.030 -2.561 -1.048
-2.561 -1.733 2.940
-1.048 2.941 -5.262
-0.144 -0.072 -0.083
-0.071 0.033 0.234
-0.009 0.026 0.007

atensor 3 C

0.027 -0.379 -0.963
-0.379 0.957 2.664
-0.964 2.664 11.403
-0.279 -0.030 -0.065
-0.031 -0.202 0.181
-0.008 0.022 -0.010

atensor 4 H

-0.843 0.223 -3.120
0.223 -8.967 -0.086
-3.120 -0.086 -5.287
0.058 0.006 -0.248
0.006 -0.169 -0.007
-0.027 -0.001 0.007

atensor 5 C

1.111 0.033 -2.842
0.033 -0.084 -0.079
-2.843 -0.079 11.475
-0.192 0.003 -0.192
0.003 -0.290 -0.005
-0.024 -0.001 -0.010

atensor 6 H

-8.292 2.201 -0.885
2.201 -1.467 -2.994
-0.885 -2.994 -5.261
-0.151 0.062 -0.070
0.061 0.040 -0.238

-0.008 -0.026 0.007

atensor 7 C

-0.007 0.326 -0.815
0.326 1.000 -2.715
-0.815 -2.715 11.414
-0.282 0.026 -0.055
0.026 -0.199 -0.184
-0.007 -0.023 -0.010

atensor 8 H

-3.430 -3.781 2.574
-3.781 -6.353 -1.766
2.575 -1.766 -5.274
-0.014 -0.106 0.205
-0.107 -0.098 -0.140
0.023 -0.015 0.007

atensor 9 C

0.721 -0.557 2.327
-0.557 0.290 -1.604
2.327 -1.604 11.374
-0.222 -0.046 0.159
-0.046 -0.258 -0.109
0.019 -0.013 -0.010

atensor 10 H

-3.855 3.921 2.474
3.921 -5.935 1.904
2.474 1.905 -5.278
-0.026 0.111 0.197
0.111 -0.086 0.151
0.022 0.017 0.007

atensor 11 C

0.667 0.576 2.237
0.576 0.359 1.728
2.237 1.728 11.392
-0.227 0.048 0.152
0.048 -0.253 0.117
0.018 0.014 -0.010

atensor 12 H

-8.286 2.201 0.885
2.201 -1.466 2.995
0.885 2.995 -5.255
-0.151 0.062 0.070
0.061 0.040 0.238
0.008 0.026 0.007

atensor 13 C

-0.008 0.326 0.816
0.326 0.999 2.713
0.816 2.713 11.405
-0.282 0.026 0.055
0.026 -0.199 0.184
0.007 0.023 -0.010

atensor 14 H

-3.435 -3.782 -2.574
-3.782 -6.359 1.766
-2.575 1.766 -5.278
-0.014 -0.106 -0.205
-0.107 -0.098 0.140
-0.023 0.015 0.007

atensor 15 C

0.722 -0.556 -2.326
-0.556 0.290 1.602
-2.326 1.602 11.389
-0.222 -0.046 -0.158
-0.046 -0.258 0.109
-0.019 0.013 -0.010

atensor 16 H
-3.856 3.921 -2.473
3.921 -5.934 -1.904
-2.473 -1.904 -5.278
-0.026 0.110 -0.197
0.111 -0.086 -0.151
-0.022 -0.017 0.007

atensor 17 C
0.661 0.576 -2.235
0.576 0.356 -1.728
-2.235 -1.728 11.393
-0.227 0.048 -0.152
0.047 -0.253 -0.117
-0.019 -0.014 -0.010

atensor 18 H
-8.028 -2.561 1.047
-2.561 -1.731 -2.940
1.048 -2.941 -5.261
-0.144 -0.072 0.083
-0.071 0.033 -0.234
0.009 -0.026 0.007

atensor 19 C
0.027 -0.379 0.963
-0.379 0.957 -2.664
0.963 -2.664 11.400
-0.279 -0.030 0.065
-0.031 -0.202 -0.181
0.008 -0.022 -0.010

atensor 20 C
1.117 0.033 2.842
0.033 -0.078 0.078
2.842 0.078 11.470
-0.192 0.003 0.192
0.003 -0.290 0.005
0.024 0.001 -0.010

atensor 21 H
-0.841 0.223 3.120
0.223 -8.963 0.085
3.121 0.085 -5.283
0.058 0.006 0.248
0.006 -0.169 0.007
0.027 0.001 0.007

orbtensor 1 Ni
-12239.940 -504.391 58.109
-504.391 -11603.808 -20.898
58.109 -20.898 -177.527
2272.970 -0.002 0.002
-0.002 2272.968 0.000
0.002 0.000 2278.876

orbtensor 2 H
3.764 5.528 1.114
5.528 -10.129 -3.022
1.114 -3.022 3.146

24.814	-5.737	-0.996
-5.737	38.931	2.798
-0.996	2.798	24.049

orbtensor 3 C

-151.423	13.630	7.335
13.630	-185.178	-20.219
7.335	-20.219	-58.045
259.730	6.977	-1.154
6.977	242.718	3.279
-1.154	3.279	242.880

orbtensor 4 H

-11.976	-0.448	3.623
-0.448	5.121	0.148
3.623	0.148	3.195
40.929	0.498	-2.968
0.498	22.783	-0.081
-2.968	-0.081	24.041

orbtensor 5 C

-186.721	1.942	25.834
1.942	-141.813	0.636
25.834	0.636	-58.532
240.130	-0.611	-3.452
-0.611	262.221	-0.090
-3.452	-0.090	242.885

orbtensor 6 H

4.204	-4.652	1.071
-4.652	-10.877	3.087
1.071	3.087	3.281
24.221	4.928	-0.841
4.928	39.511	-2.849
-0.841	-2.849	24.043

orbtensor 7 C

-146.960	-6.912	5.635
-6.912	-190.011	21.393
5.635	21.393	-59.950
260.420	-6.011	-0.971
-6.011	241.972	-3.336
-0.971	-3.336	242.862

orbtensor 8 H

-6.194	8.147	-2.875
8.147	-0.180	1.805
-2.875	1.805	3.300
35.151	-8.484	2.443
-8.484	28.585	-1.676
2.443	-1.676	24.043

orbtensor 9 C

-169.516	21.297	-19.808
21.297	-163.089	13.771
-19.808	13.771	-57.950
247.276	10.252	2.863
10.252	255.200	-1.958
2.863	-1.958	242.858

orbtensor 10 H

-5.598	-8.449	-2.914
-8.449	-1.408	-1.994
-2.914	-1.994	3.213
34.192	8.793	2.347
8.793	29.525	1.806
2.347	1.806	24.032

orbtensor 11 C
-170.014 -22.390 -18.975
-22.390 -163.142 -15.727
-18.975 -15.727 -58.691
248.414 -10.631 2.746
-10.631 254.055 2.110
2.746 2.110 242.836

orbtensor 12 H
4.175 -4.576 -1.154
-4.576 -10.751 -3.351
-1.154 -3.351 3.004
24.222 4.928 0.840
4.928 39.510 2.851
0.840 2.851 24.044

orbtensor 13 C
-150.319 -7.811 -8.321
-7.811 -188.023 -24.029
-8.321 -24.029 -52.509
260.418 -6.014 0.963
-6.014 241.970 3.336
0.963 3.336 242.864

orbtensor 14 H
-6.318 8.221 2.739
8.221 -0.224 -1.715
2.739 -1.715 2.936
35.152 -8.484 -2.446
-8.484 28.586 1.677
-2.446 1.677 24.043

orbtensor 15 C
-169.114 23.393 18.406
23.393 -160.912 -13.138
18.406 -13.138 -54.382
247.285 10.252 -2.863
10.252 255.206 1.954
-2.863 1.954 242.856

orbtensor 16 H
-5.582 -8.372 2.756
-8.372 -1.260 2.258
2.756 2.258 3.039
34.194 8.792 -2.348
8.792 29.526 -1.807
-2.348 -1.807 24.031

orbtensor 17 C
-168.796 -19.990 18.046
-19.990 -165.189 14.906
18.046 14.906 -53.598
248.424 -10.631 -2.749
-10.631 254.060 -2.107
-2.749 -2.107 242.829

orbtensor 18 H
3.656 5.617 -1.043
5.617 -10.123 3.136
-1.043 3.136 3.159
24.814 -5.735 0.994
-5.735 38.933 -2.797
0.994 -2.797 24.049

orbtensor 19 C
-149.548 12.137 -6.512

```

12.137 -188.769 24.211
-6.512 24.211 -54.612
259.723 6.984 1.147
6.984 242.716 -3.279
1.147 -3.279 242.873

```

```

orbtensor 20 C
-187.201 -0.877 -22.000
-0.877 -141.846 -2.039
-22.000 -2.039 -53.455
240.124 -0.613 3.452
-0.613 262.217 0.092
3.452 0.092 242.894

```

```

orbtensor 21 H
-12.088 -0.388 -3.391
-0.388 5.206 -0.296
-3.391 -0.296 3.108
40.928 0.497 2.969
0.497 22.784 0.081
2.969 0.081 24.043

```

```

gtensor (ppt)
-0.084 0.000 0.000
0.000 -0.084 0.000
0.000 0.000 -0.226
94.123 4.676 -0.539
4.676 88.266 0.194
-0.539 0.194 -0.256

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	36.0707	-5732.15367	29337.59987	462.40763	29800.00750	24067.85383
2	H	-5.0430	28.19167	367.16676	0.25635	367.42311	395.61478
3	C	3.9653	116.89400	-1147.91840	32.03971	-1115.87869	-998.98469
4	H	-5.0670	28.03100	368.91413	-0.58333	368.33081	396.36181
5	C	4.0033	119.39000	-1158.91896	31.62875	-1127.29021	-1007.90021
6	H	-5.0413	28.12767	367.04542	-0.23381	366.81160	394.93927
7	C	3.9720	116.11100	-1149.84832	31.84563	-1118.00269	-1001.89169
8	H	-5.0540	28.23500	367.96764	0.13711	368.10475	396.33975
9	C	3.9650	118.25967	-1147.82190	32.05228	-1115.76962	-997.50995
10	H	-5.0577	27.98533	368.23460	-0.72353	367.51107	395.49641
11	C	3.9760	117.81933	-1151.00627	31.49622	-1119.51005	-1001.69072
12	H	-5.0370	28.06800	366.72992	-0.23730	366.49262	394.56062
13	C	3.9683	118.13367	-1148.78686	31.80588	-1116.98098	-998.84732
14	H	-5.0590	28.05833	368.33168	0.05324	368.38491	396.44325
15	C	3.9703	120.31300	-1149.36584	31.78914	-1117.57670	-997.26370
16	H	-5.0577	27.98267	368.23460	-0.77077	367.46383	395.44650
17	C	3.9733	119.24333	-1150.23431	31.34356	-1118.89074	-999.64741
18	H	-5.0413	28.16267	367.04542	0.31140	367.35682	395.51949
19	C	3.9643	117.46100	-1147.62891	32.23235	-1115.39656	-997.93556
20	C	4.0057	120.91100	-1159.59443	31.89191	-1127.70253	-1006.79153
21	H	-5.0637	27.99367	368.67144	-0.50073	368.17072	396.16439
	C Average	3.9764	118.45360	-1151.11242	31.81254	-1119.29988	-1000.84628
	H Average	-5.0522	28.08360	367.83416	-0.22914	367.60503	395.68863

3NiCp2-STO-PBE0-DZ-TZ2P

Temperature: 298
Spin: 1

atensor 1 Ni
98.570 0.002 0.002
0.002 98.592 0.009
0.002 0.009 2.565
-40.910 0.001 -0.003
0.001 -40.901 -0.003
-0.003 -0.003 -2.890

atensor 2 H
-7.178 -2.527 -1.046
-2.527 -0.969 2.939
-1.046 2.939 -3.735
-0.131 -0.062 -0.075
-0.062 0.022 0.212
-0.009 0.025 0.010

atensor 3 C
1.245 -0.331 -0.995
-0.331 2.059 2.792
-0.995 2.792 13.123
-0.287 -0.033 -0.063
-0.033 -0.205 0.177
-0.006 0.018 -0.011

atensor 4 H
-0.078 0.220 -3.118
0.220 -8.077 -0.085
-3.118 -0.085 -3.737
0.044 0.005 -0.225
0.005 -0.153 -0.006
-0.026 -0.001 0.010

atensor 5 C
2.190 0.028 -2.965
0.028 1.143 -0.080
-2.965 -0.080 13.158
-0.193 0.003 -0.188
0.003 -0.298 -0.005
-0.019 -0.001 -0.011

atensor 6 H
-7.436 2.171 -0.883
2.171 -0.710 -2.992
-0.883 -2.992 -3.736
-0.137 0.053 -0.064
0.053 0.028 -0.216
-0.007 -0.025 0.010

atensor 7 C
1.212 0.285 -0.839
0.285 2.094 -2.843
-0.839 -2.843 13.121
-0.290 0.029 -0.053
0.029 -0.201 -0.180
-0.005 -0.018 -0.011

atensor 8 H
-2.627 -3.733 2.573
-3.733 -5.514 -1.764
2.574 -1.764 -3.731
-0.019 -0.092 0.186
-0.092 -0.090 -0.127
0.022 -0.015 0.010

atensor 9 C
1.840 -0.490 2.445
-0.490 1.462 -1.677
2.445 -1.677 13.116
-0.227 -0.049 0.155
-0.049 -0.265 -0.106
0.016 -0.011 -0.011

atensor 10 H
-3.047 3.869 2.473
3.869 -5.101 1.902
2.473 1.902 -3.735
-0.029 0.095 0.178
0.095 -0.080 0.137
0.021 0.016 0.010

atensor 11 C
1.790 0.507 2.351
0.507 1.520 1.808
2.351 1.808 13.128
-0.232 0.051 0.149
0.051 -0.259 0.114
0.015 0.012 -0.010

atensor 12 H
-7.432 2.171 0.883
2.171 -0.710 2.993
0.883 2.993 -3.732
-0.137 0.053 0.064
0.053 0.028 0.216
0.007 0.025 0.010

atensor 13 C
1.210 0.284 0.840
0.284 2.092 2.841
0.840 2.841 13.110
-0.290 0.029 0.053
0.029 -0.201 0.180
0.005 0.018 -0.011

atensor 14 H
-2.631 -3.734 -2.573
-3.734 -5.519 1.763
-2.573 1.763 -3.734
-0.019 -0.092 -0.186
-0.092 -0.090 0.127
-0.022 0.015 0.010

atensor 15 C
1.843 -0.489 -2.445
-0.489 1.465 1.675
-2.445 1.675 13.134
-0.227 -0.049 -0.155
-0.049 -0.265 0.106
-0.016 0.011 -0.011

atensor 16 H
-3.048 3.869 -2.472
3.869 -5.100 -1.902
-2.472 -1.902 -3.735
-0.029 0.095 -0.178
0.095 -0.080 -0.137
-0.021 -0.016 0.010

atensor 17 C
1.783 0.508 -2.349
0.508 1.515 -1.808

-2.349 -1.809 13.128
-0.232 0.051 -0.149
0.051 -0.259 -0.114
-0.015 -0.012 -0.011

atensor 18 H
-7.176 -2.527 1.045
-2.527 -0.968 -2.939
1.045 -2.939 -3.734
-0.131 -0.062 0.075
-0.062 0.022 -0.212
0.009 -0.025 0.010

atensor 19 C
1.245 -0.332 0.995
-0.332 2.058 -2.792
0.995 -2.793 13.118
-0.287 -0.033 0.063
-0.033 -0.205 -0.177
0.006 -0.018 -0.011

atensor 20 C
2.199 0.029 2.965
0.029 1.152 0.080
2.965 0.080 13.154
-0.193 0.003 0.188
0.003 -0.298 0.005
0.019 0.000 -0.011

atensor 21 H
-0.076 0.219 3.119
0.219 -8.072 0.085
3.119 0.085 -3.734
0.044 0.005 0.225
0.005 -0.153 0.006
0.026 0.001 0.010

orbtensor 1 Ni
-11269.892 -287.962 41.908
-287.962-11420.326 -60.529
41.908 -60.529 -289.786
2276.870 0.001 0.002
0.001 2276.865 -0.001
0.002 -0.001 2279.380

orbtensor 2 H
0.390 5.184 1.335
5.184 -12.542 -3.830
1.335 -3.830 -0.198
26.942 -4.981 -1.195
-4.981 39.185 3.359
-1.195 3.359 25.090

orbtensor 3 C
-171.443 13.113 8.087
13.113 -210.189 -20.377
8.087 -20.377 -67.481
249.927 2.494 -2.216
2.494 243.809 6.223
-2.216 6.223 233.029

orbtensor 4 H
-14.376 -0.513 4.179
-0.513 1.927 0.111
4.179 0.111 -0.130
40.946 0.433 -3.563
0.433 25.183 -0.098

```

-3.563   -0.098   25.090

orbtensor 5 C
-214.881  -0.604   24.691
-0.604  -163.130   2.906
24.691   2.906  -67.303
242.936  -0.217  -6.603
-0.217  250.817  -0.180
-6.603   -0.180  233.037

orbtensor 6 H
0.801   -4.373   1.250
-4.373  -13.116   3.807
1.250   3.807  -0.135
26.433   4.281  -1.008
4.281   39.694  -3.419
-1.008  -3.419   25.090

orbtensor 7 C
-169.186  -10.718   4.786
-10.718  -211.547  22.205
4.786   22.205  -66.804
250.177  -2.143  -1.870
-2.143  243.548  -6.335
-1.870  -6.335  233.026

orbtensor 8 H
-9.012   7.623  -3.349
7.623  -3.136   2.355
-3.349   2.355  -0.154
35.908  -7.362   2.941
-7.362  30.215  -2.016
2.941  -2.016   25.089

orbtensor 9 C
-194.491  23.469  -20.342
23.469 -182.844  12.322
-20.342  12.322  -66.608
245.435   3.680   5.451
3.680  248.289  -3.734
5.451  -3.734  233.032

orbtensor 10 H
-8.117  -7.829  -3.400
-7.829  -4.226  -2.490
-3.400  -2.490  -0.208
35.086   7.629   2.826
7.629  31.038   2.174
2.826   2.174   25.090

orbtensor 11 C
-192.127  -24.014  -17.654
-24.014 -183.893  -16.346
-17.654  -16.346  -67.280
245.850  -3.814   5.237
-3.814  247.874   4.030
5.237   4.030  233.030

orbtensor 12 H
0.582   -4.277  -1.153
-4.277  -13.109  -3.741
-1.153  -3.741  -0.130
26.433   4.281   1.008
4.281   39.693   3.421
1.008   3.421   25.091

orbtensor 13 C

```

-171.211	-11.722	-6.543
-11.722	-208.524	-23.439
-6.543	-23.439	-70.851
250.173	-2.145	1.863
-2.145	243.546	6.339
1.863	6.339	233.027

orbtensor 14 H

-9.312	7.571	3.031
7.571	-3.403	-2.007
3.031	-2.007	-0.205
35.910	-7.361	-2.943
-7.361	30.216	2.016
-2.943	2.016	25.090

orbtensor 15 C

-197.008	25.000	18.090
25.000	-181.000	-11.790
18.090	-11.790	-70.847
245.445	3.682	-5.454
3.682	248.293	3.733
-5.454	3.733	233.033

orbtensor 16 H

-8.191	-7.768	2.885
-7.768	-4.294	2.436
2.885	2.436	-0.004
35.088	7.629	-2.827
7.629	31.043	-2.174
-2.827	-2.174	25.091

orbtensor 17 C

-191.410	-21.378	17.598
-21.378	-184.726	14.609
17.598	14.609	-71.221
245.856	-3.812	-5.241
-3.812	247.889	-4.026
-5.241	-4.026	233.030

orbtensor 18 H

-0.043	5.119	-1.165
5.119	-12.606	3.649
-1.165	3.649	0.192
26.943	-4.982	1.193
-4.982	39.186	-3.358
1.193	-3.358	25.089

orbtensor 19 C

-168.338	12.685	-8.951
12.685	-210.608	21.704
-8.951	21.704	-71.901
249.929	2.492	2.206
2.492	243.806	-6.225
2.206	-6.225	233.027

orbtensor 20 C

-212.289	-3.076	-20.153
-3.076	-162.405	-1.179
-20.153	-1.179	-71.908
242.926	-0.213	6.602
-0.213	250.809	0.181
6.602	0.181	233.036

orbtensor 21 H

-14.411	-0.479	-3.728
-0.479	1.690	-0.134
-3.728	-0.134	0.102


```

40.944    0.433    3.563
0.433    25.181    0.097
3.563     0.097    25.089

```

```

gtensor (ppt)
-0.090    0.000    0.000
0.000    -0.090    0.000
0.000     0.000   -0.226
84.141    2.688   -0.387
2.688    85.587    0.562
-0.387    0.562    0.246

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	38.3420	-5382.29633	31123.62892	430.70309	31554.33200	26172.03567
2	H	-3.9937	26.28900	290.19589	0.32718	290.52307	316.81207
3	C	5.3080	92.55067	-1533.58299	30.81127	-1502.77172	-1410.22105
4	H	-3.9970	26.21333	290.43810	0.29633	290.73444	316.94777
5	C	5.3297	93.82533	-1539.84291	30.91653	-1508.92638	-1415.10105
6	H	-3.9937	26.25567	290.19589	0.10041	290.29630	316.55197
7	C	5.3083	93.07133	-1533.67930	30.94144	-1502.73786	-1409.66653
8	H	-3.9903	26.30333	289.95368	0.58427	290.53795	316.84128
9	C	5.3050	94.27100	-1532.71623	31.25586	-1501.46038	-1407.18938
10	H	-3.9940	26.22100	290.22011	0.03268	290.25279	316.47379
11	C	5.3123	94.48467	-1534.83498	30.80528	-1504.02970	-1409.54503
12	H	-3.9910	26.18667	290.00212	0.03617	290.03829	316.22496
13	C	5.3033	92.05333	-1532.23470	30.67153	-1501.56317	-1409.50984
14	H	-3.9943	26.09867	290.24433	0.48807	290.73240	316.83107
15	C	5.3130	92.63867	-1535.02759	30.92962	-1504.09797	-1411.45930
16	H	-3.9940	26.24433	290.22011	0.03814	290.25826	316.50259
17	C	5.3080	93.13933	-1533.58299	30.83884	-1502.74415	-1409.60482
18	H	-3.9923	26.25367	290.09900	0.42752	290.52653	316.78019
19	C	5.3060	91.97167	-1533.00515	31.17808	-1501.82707	-1409.85541
20	C	5.3343	93.38967	-1541.19120	31.09541	-1510.09579	-1416.70612
21	H	-3.9937	26.19833	290.19589	0.35278	290.54867	316.74700
C Average		5.3128	93.13957	-1534.96980	30.94439	-1504.02542	-1410.88585
H Average		-3.9934	26.22640	290.17651	0.26836	290.44487	316.67127

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3NiCp2-STO-PBE0-DZ-QZ4P
Temperature: 298
Spin: 1

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```

atensor 1 Ni
99.206 0.002 0.002
0.002 99.230 0.007
0.002 0.007 3.179
-40.453 0.000 -0.003
0.000 -40.445 -0.002
-0.003 -0.002 -2.895

```

```

atensor 2 H
-6.880 -2.507 -1.044
-2.507 -0.721 2.934
-1.044 2.934 -3.535
-0.131 -0.061 -0.074
-0.061 0.018 0.207
-0.009 0.024 0.010

```

atensor 3 C
0.840 -0.335 -1.012
-0.335 1.663 2.840
-1.012 2.840 13.058
-0.290 -0.032 -0.062
-0.032 -0.212 0.175
-0.006 0.018 -0.011

atensor 4 H
0.165 0.218 -3.113
0.218 -7.769 -0.085
-3.113 -0.085 -3.535
0.040 0.005 -0.220
0.005 -0.152 -0.006
-0.026 -0.001 0.010

atensor 5 C
1.794 0.029 -3.017
0.029 0.735 -0.082
-3.017 -0.082 13.090
-0.201 0.003 -0.186
0.003 -0.302 -0.005
-0.019 -0.001 -0.011

atensor 6 H
-7.137 2.154 -0.881
2.154 -0.466 -2.987
-0.881 -2.987 -3.536
-0.137 0.052 -0.062
0.052 0.025 -0.211
-0.007 -0.025 0.010

atensor 7 C
0.810 0.288 -0.854
0.288 1.703 -2.892
-0.854 -2.892 13.059
-0.294 0.027 -0.053
0.027 -0.209 -0.178
-0.005 -0.018 -0.011

atensor 8 H
-2.364 -3.703 2.569
-3.703 -5.228 -1.761
2.569 -1.761 -3.529
-0.021 -0.090 0.182
-0.090 -0.091 -0.125
0.021 -0.015 0.010

atensor 9 C
1.446 -0.495 2.488
-0.495 1.063 -1.705
2.488 -1.705 13.054
-0.233 -0.047 0.154
-0.047 -0.269 -0.105
0.016 -0.011 -0.011

atensor 10 H
-2.781 3.838 2.469
3.838 -4.819 1.899
2.469 1.899 -3.533
-0.032 0.093 0.175
0.093 -0.081 0.134
0.020 0.016 0.010

atensor 11 C
1.392 0.513 2.391

0.513 1.120 1.839
2.391 1.839 13.063
-0.238 0.049 0.148
0.049 -0.264 0.113
0.015 0.011 -0.011

atensor 12 H
-7.133 2.154 0.881
2.154 -0.465 2.988
0.881 2.988 -3.533
-0.137 0.052 0.062
0.052 0.025 0.211
0.007 0.025 0.010

atensor 13 C
0.810 0.288 0.854
0.288 1.701 2.890
0.855 2.890 13.051
-0.294 0.027 0.053
0.027 -0.209 0.178
0.005 0.018 -0.011

atensor 14 H
-2.368 -3.704 -2.569
-3.704 -5.233 1.760
-2.569 1.761 -3.532
-0.022 -0.090 -0.182
-0.090 -0.091 0.124
-0.021 0.014 0.010

atensor 15 C
1.446 -0.495 -2.487
-0.495 1.063 1.704
-2.487 1.704 13.071
-0.233 -0.047 -0.153
-0.047 -0.269 0.105
-0.016 0.011 -0.011

atensor 16 H
-2.783 3.838 -2.468
3.838 -4.819 -1.899
-2.468 -1.899 -3.534
-0.032 0.093 -0.175
0.093 -0.081 -0.134
-0.020 -0.016 0.010

atensor 17 C
1.391 0.513 -2.389
0.513 1.119 -1.840
-2.389 -1.840 13.070
-0.238 0.049 -0.147
0.049 -0.264 -0.113
-0.015 -0.011 -0.011

atensor 18 H
-6.878 -2.507 1.043
-2.507 -0.720 -2.934
1.043 -2.934 -3.534
-0.131 -0.061 0.074
-0.061 0.018 -0.208
0.009 -0.024 0.010

atensor 19 C
0.839 -0.336 1.012
-0.336 1.663 -2.840
1.012 -2.840 13.054
-0.290 -0.032 0.062

-0.032 -0.212 -0.175
0.006 -0.018 -0.011

atensor 20 C
1.797 0.029 3.016
0.029 0.738 0.081
3.016 0.081 13.079
-0.201 0.003 0.186
0.003 -0.302 0.005
0.019 0.000 -0.011

atensor 21 H
0.167 0.217 3.114
0.217 -7.764 0.085
3.114 0.085 -3.530
0.040 0.005 0.220
0.005 -0.152 0.006
0.026 0.001 0.010

orbtensor 1 Ni
-11065.366 492.891 -12.890
492.891-11189.326 -99.479
-12.890 -99.479 -812.054
2255.128 0.001 0.005
0.001 2255.119 -0.002
0.005 -0.002 2281.579

orbtensor 2 H
2.497 6.819 1.195
6.819 -14.378 -2.986
1.195 -2.986 1.433
24.233 -6.641 -0.982
-6.641 40.553 2.762
-0.982 2.762 23.027

orbtensor 3 C
-180.053 17.791 8.007
17.791 -227.851 -19.913
8.007 -19.913 -73.195
252.814 -0.558 -1.822
-0.558 254.193 5.119
-1.822 5.119 231.592

orbtensor 4 H
-17.084 -0.585 3.309
-0.585 5.339 0.011
3.309 0.011 1.460
42.900 0.577 -2.930
0.577 21.889 -0.080
-2.930 -0.080 23.027

orbtensor 5 C
-238.530 -4.892 24.072
-4.892 -182.163 -1.046
24.072 -1.046 -73.138
254.399 0.051 -5.432
0.051 252.628 -0.148
-5.432 -0.148 231.598

orbtensor 6 H
3.381 -6.124 0.715
-6.124 -14.964 2.912
0.715 2.912 1.532
23.555 5.707 -0.829
5.707 41.232 -2.811
-0.829 -2.811 23.027

orbtensor 7 C
-184.217 -20.418 5.712
-20.418 -227.662 20.542
5.712 20.542 -72.610
252.757 0.479 -1.538
0.479 254.249 -5.210
-1.538 -5.210 231.591

orbtensor 8 H
-10.170 10.258 -2.773
10.258 -2.007 1.864
-2.773 1.864 1.538
36.188 -9.813 2.418
-9.813 28.597 -1.657
2.418 -1.657 23.027

orbtensor 9 C
-222.985 26.553 -18.205
26.553 -192.304 14.209
-18.205 14.209 -73.216
253.821 -0.828 4.480
-0.828 253.183 -3.071
4.480 -3.071 231.594

orbtensor 10 H
-8.687 -10.802 -2.505
-10.802 -2.674 -1.817
-2.505 -1.817 1.483
35.090 10.169 2.324
10.169 29.695 1.788
2.324 1.788 23.027

orbtensor 11 C
-218.165 -25.739 -19.476
-25.739 -200.716 -12.810
-19.476 -12.810 -73.974
253.722 0.859 4.304
0.859 253.273 3.315
4.304 3.315 231.590

orbtensor 12 H
3.408 -6.074 -1.068
-6.074 -14.633 -3.659
-1.068 -3.659 1.169
23.556 5.707 0.829
5.707 41.232 2.814
0.829 2.814 23.028

orbtensor 13 C
-179.543 -19.091 -7.843
-19.091 -227.848 -23.263
-7.843 -23.263 -68.298
252.757 0.480 1.533
0.480 254.247 5.212
1.533 5.212 231.592

orbtensor 14 H
-9.698 10.188 3.177
10.188 -1.594 -2.443
3.177 -2.443 1.155
36.187 -9.812 -2.421
-9.812 28.598 1.659
-2.421 1.659 23.027

orbtensor 15 C
-220.342 22.804 21.777
22.804 -191.514 -11.419

21.777	-11.419	-67.621
253.821	-0.828	-4.484
-0.828	253.184	3.072
-4.484	3.072	231.593

orbtensor 16 H

-8.429	-10.680	2.931
-10.680	-2.576	2.157
2.931	2.157	1.255
35.090	10.169	-2.325
10.169	29.696	-1.788
-2.325	-1.788	23.026

orbtensor 17 C

-218.229	-27.551	19.595
-27.551	-197.488	11.723
19.595	11.723	-66.869
253.723	0.858	-4.309
0.858	253.273	-3.311
-4.309	-3.311	231.586

orbtensor 18 H

2.730	6.750	-1.287
6.750	-13.974	3.710
-1.287	3.710	1.328
24.233	-6.640	0.981
-6.640	40.555	-2.761
0.981	-2.761	23.027

orbtensor 19 C

-181.511	19.214	-11.305
19.214	-222.083	24.225
-11.305	24.225	-67.646
252.812	-0.557	1.816
-0.557	254.199	-5.118
1.816	-5.118	231.593

orbtensor 20 C

-235.873	-2.106	-22.118
-2.106	-182.402	-0.210
-22.118	-0.210	-67.479
254.402	0.047	5.429
0.047	252.630	0.149
5.429	0.149	231.603

orbtensor 21 H

-16.698	-0.633	-3.812
-0.633	5.576	0.193
-3.812	0.193	1.280
42.900	0.576	2.930
0.576	21.889	0.080
2.930	0.080	23.027

gtensor (ppt)

-0.114	0.000	0.000
0.000	-0.114	0.000
0.000	0.000	-0.232
82.102	-4.583	0.123
-4.583	83.175	0.924
0.123	0.924	5.076

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	39.2740	-5424.97333	31881.84550	398.04994	32279.89545	26854.92212
2	H	-3.7463	25.78833	272.23798	-0.17762	272.06036	297.84869
3	C	5.0160	85.83333	-1449.29485	28.76014	-1420.53471	-1334.70137
4	H	-3.7470	25.84367	272.28642	0.28951	272.57593	298.41960
5	C	5.0350	81.59800	-1454.78460	29.31522	-1425.46938	-1343.87138
6	H	-3.7470	25.92100	272.28642	0.46688	272.75330	298.67430
7	C	5.0193	84.70267	-1450.25796	29.55258	-1420.70539	-1336.00272
8	H	-3.7410	25.72433	271.85042	-0.15554	271.69488	297.41921
9	C	5.0167	83.36433	-1449.48747	29.06588	-1420.42160	-1337.05726
10	H	-3.7453	25.97800	272.16531	0.58991	272.75522	298.73322
11	C	5.0207	81.91000	-1450.64321	29.23878	-1421.40443	-1339.49443
12	H	-3.7443	25.92000	272.09264	0.32687	272.41951	298.33951
13	C	5.0160	87.63567	-1449.29485	28.99858	-1420.29627	-1332.66060
14	H	-3.7453	25.89167	272.16531	-0.21855	271.94676	297.83843
15	C	5.0223	86.37367	-1451.12477	28.86154	-1422.26323	-1335.88956
16	H	-3.7463	26.02067	272.23798	0.69058	272.92856	298.94923
17	C	5.0223	85.33200	-1451.12477	29.64378	-1421.48098	-1336.14898
18	H	-3.7450	25.96633	272.14109	-0.05159	272.08950	298.05583
19	C	5.0143	89.12133	-1448.81329	29.23482	-1419.57847	-1330.45714
20	C	5.0333	84.29367	-1454.30304	29.19496	-1425.10808	-1340.81441
21	H	-3.7430	25.99133	271.99575	0.26771	272.26346	298.25480
C Average		5.0216	85.01647	-1450.91288	29.18663	-1421.72625	-1336.70979
H Average		-3.7451	25.90453	272.14593	0.20282	272.34875	298.25328

3NiCp2-STO-PBE0-TZ2P-DZ
Temperature: 298
Spin: 1

atensor 1 Ni
97.145 0.016 0.002
0.016 97.087 0.010
0.002 0.010 -0.496
-41.365 -0.003 -0.003
-0.003 -41.344 -0.003
-0.003 -0.003 -2.832

atensor 2 H
-7.895 -2.542 -1.059
-2.542 -1.644 2.971
-1.059 2.971 -5.121
-0.147 -0.074 -0.084
-0.074 0.035 0.236
-0.009 0.025 0.007

atensor 3 C
0.155 -0.379 -0.967
-0.379 1.087 2.678
-0.967 2.678 11.290
-0.277 -0.032 -0.065
-0.032 -0.197 0.182
-0.007 0.021 -0.009

atensor 4 H
-0.760 0.221 -3.152
0.221 -8.822 -0.087
-3.152 -0.087 -5.144
0.061 0.006 -0.251
0.006 -0.173 -0.007
-0.026 -0.001 0.007

atensor 5 C

1.243 0.033 -2.857
0.033 0.045 -0.079
-2.857 -0.079 11.360
-0.187 0.003 -0.194
0.003 -0.289 -0.005
-0.022 -0.001 -0.009

atensor 6 H
-8.154 2.185 -0.894
2.185 -1.380 -3.025
-0.894 -3.025 -5.119
-0.154 0.063 -0.071
0.063 0.042 -0.240
-0.007 -0.025 0.007

atensor 7 C
0.121 0.327 -0.818
0.327 1.130 -2.730
-0.818 -2.730 11.301
-0.280 0.027 -0.055
0.027 -0.194 -0.186
-0.006 -0.021 -0.009

atensor 8 H
-3.330 -3.754 2.601
-3.754 -6.232 -1.784
2.601 -1.784 -5.135
-0.014 -0.109 0.207
-0.109 -0.098 -0.142
0.022 -0.015 0.007

atensor 9 C
0.851 -0.558 2.339
-0.558 0.419 -1.612
2.340 -1.612 11.266
-0.218 -0.048 0.160
-0.047 -0.255 -0.109
0.018 -0.012 -0.009

atensor 10 H
-3.753 3.892 2.499
3.892 -5.817 1.924
2.499 1.924 -5.139
-0.026 0.113 0.199
0.113 -0.086 0.153
0.021 0.016 0.007

atensor 11 C
0.797 0.577 2.249
0.577 0.489 1.736
2.249 1.737 11.285
-0.223 0.050 0.154
0.049 -0.250 0.118
0.017 0.013 -0.009

atensor 12 H
-8.148 2.184 0.894
2.184 -1.379 3.026
0.894 3.026 -5.113
-0.154 0.063 0.071
0.063 0.042 0.240
0.007 0.025 0.007

atensor 13 C
0.121 0.326 0.819
0.326 1.129 2.727
0.819 2.727 11.292

-0.280 0.027 0.055
0.027 -0.194 0.186
0.006 0.021 -0.009

atensor 14 H
-3.335 -3.755 -2.601
-3.755 -6.237 1.784
-2.601 1.784 -5.139
-0.014 -0.109 -0.207
-0.109 -0.098 0.142
-0.022 0.015 0.007

atensor 15 C
0.852 -0.557 -2.339
-0.557 0.419 1.610
-2.339 1.610 11.281
-0.218 -0.048 -0.160
-0.047 -0.255 0.109
-0.018 0.012 -0.009

atensor 16 H
-3.753 3.892 -2.499
3.892 -5.817 -1.923
-2.499 -1.924 -5.140
-0.026 0.113 -0.199
0.113 -0.086 -0.153
-0.021 -0.016 0.007

atensor 17 C
0.792 0.577 -2.247
0.577 0.486 -1.737
-2.247 -1.737 11.287
-0.223 0.049 -0.153
0.049 -0.250 -0.118
-0.017 -0.013 -0.009

atensor 18 H
-7.893 -2.542 1.058
-2.542 -1.643 -2.971
1.058 -2.971 -5.120
-0.147 -0.074 0.084
-0.074 0.035 -0.236
0.009 -0.025 0.007

atensor 19 C
0.155 -0.380 0.966
-0.380 1.087 -2.678
0.966 -2.679 11.286
-0.277 -0.032 0.065
-0.032 -0.197 -0.182
0.007 -0.021 -0.009

atensor 20 C
1.250 0.033 2.857
0.033 0.051 0.078
2.857 0.078 11.355
-0.187 0.003 0.194
0.003 -0.289 0.005
0.022 0.001 -0.009

atensor 21 H
-0.758 0.221 3.153
0.221 -8.818 0.086
3.153 0.086 -5.140
0.061 0.006 0.251
0.006 -0.173 0.007
0.026 0.001 0.007

orbtensor 1 Ni
-11104.592 -18.661 63.247
-18.661-11785.619 -20.500
63.247 -20.500 -646.761
2273.321 -0.002 0.002
-0.002 2273.322 0.000
0.002 0.000 2279.323

orbtensor 2 H
3.676 5.485 1.050
5.485 -10.297 -3.390
1.050 -3.390 3.227
24.830 -5.758 -1.035
-5.758 38.990 2.906
-1.035 2.906 23.982

orbtensor 3 C
-154.575 11.708 6.989
11.708 -185.480 -21.925
6.989 -21.925 -57.942
258.917 6.793 -1.227
6.793 242.345 3.472
-1.227 3.472 243.085

orbtensor 4 H
-12.152 -0.368 3.541
-0.368 5.514 -0.080
3.541 -0.080 3.269
40.997 0.500 -3.084
0.500 22.788 -0.085
-3.084 -0.085 23.971

orbtensor 5 C
-190.809 0.555 25.007
0.555 -142.713 0.333
25.007 0.333 -58.698
239.825 -0.595 -3.664
-0.595 261.337 -0.097
-3.664 -0.097 243.082

orbtensor 6 H
4.048 -4.870 1.083
-4.870 -11.018 3.323
1.083 3.323 3.357
24.235 4.946 -0.874
4.946 39.572 -2.959
-0.874 -2.959 23.975

orbtensor 7 C
-150.262 -8.978 5.238
-8.978 -192.199 22.344
5.238 22.344 -59.836
259.587 -5.852 -1.033
-5.852 241.621 -3.534
-1.033 -3.534 243.066

orbtensor 8 H
-6.292 8.266 -2.788
8.266 -0.162 2.170
-2.788 2.170 3.371
35.198 -8.510 2.536
-8.510 28.615 -1.741
2.536 -1.741 23.978

orbtensor 9 C
-172.828 19.671 -18.960

19.671	-163.209	14.945
-18.960	14.945	-57.893
246.783	9.989	3.025
9.989	254.507	-2.074
3.025	-2.074	243.066

orbtensor 10 H

-5.737	-8.609	-2.853
-8.609	-1.176	-2.000
-2.853	-2.000	3.295
34.236	8.818	2.436
8.818	29.558	1.876
2.436	1.876	23.967

orbtensor 11 C

-172.688	-24.411	-18.381
-24.411	-164.381	-15.601
-18.381	-15.601	-58.797
247.893	-10.359	2.901
-10.359	253.392	2.233
2.901	2.233	243.047

orbtensor 12 H

3.962	-4.767	-1.046
-4.767	-10.943	-3.265
-1.046	-3.265	3.101
24.235	4.946	0.874
4.946	39.571	2.961
0.874	2.961	23.976

orbtensor 13 C

-153.025	-8.481	-7.344
-8.481	-188.260	-23.610
-7.344	-23.610	-53.848
259.585	-5.854	1.026
-5.854	241.618	3.534
1.026	3.534	243.069

orbtensor 14 H

-6.515	8.295	2.557
8.295	-0.458	-1.903
2.557	-1.903	3.034
35.198	-8.510	-2.539
-8.510	28.616	1.741
-2.539	1.741	23.978

orbtensor 15 C

-173.002	22.260	17.628
22.260	-162.146	-13.916
17.628	-13.916	-55.579
246.792	9.989	-3.025
9.989	254.514	2.070
-3.025	2.070	243.064

orbtensor 16 H

-5.774	-8.531	2.528
-8.531	-1.178	2.057
2.528	2.057	3.132
34.239	8.818	-2.437
8.818	29.559	-1.876
-2.437	-1.876	23.967

orbtensor 17 C

-171.198	-21.606	17.218
-21.606	-166.481	13.809
17.218	13.809	-54.738
247.904	-10.360	-2.903

-10.360 253.399 -2.230
 -2.903 -2.230 243.040

orbtensor 18 H
 3.457 5.505 -1.000
 5.505 -10.381 3.223
 -1.000 3.223 3.258
 24.830 -5.756 1.034
 -5.756 38.991 -2.905
 1.034 -2.905 23.981

orbtensor 19 C
 -153.073 10.143 -7.269
 10.143 -186.624 23.971
 -7.269 23.971 -55.917
 258.911 6.799 1.221
 6.799 242.343 -3.471
 1.221 -3.471 243.078

orbtensor 20 C
 -190.873 -1.372 -20.958
 -1.372 -142.114 -0.513
 -20.958 -0.513 -54.513
 239.819 -0.597 3.665
 -0.597 261.332 0.098
 3.665 0.098 243.091

orbtensor 21 H
 -12.314 -0.321 -3.123
 -0.321 5.351 -0.083
 -3.123 -0.083 3.213
 40.996 0.499 3.085
 0.499 22.788 0.085
 3.085 0.085 23.972

gtensor (ppt)
 -0.088 0.000 0.000
 0.000 -0.088 0.000
 0.000 0.000 -0.230
 83.339 0.173 -0.586
 0.173 89.727 0.190
 -0.586 0.190 4.067

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
 Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	36.0650	-5570.33533	29309.23524	427.65908	29736.89433	24166.55899
2	H	-4.9217	28.13600	358.04262	-0.44710	357.59551	385.73151
3	C	4.0163	115.45000	-1161.74070	27.82284	-1133.91786	-1018.46786
4	H	-4.9437	28.12900	359.64308	0.07795	359.72103	387.85003
5	C	4.0543	117.34133	-1172.73235	28.22798	-1144.50437	-1027.16303
6	H	-4.9193	28.05633	357.87287	-0.45705	357.41583	385.47216
7	C	4.0230	113.99233	-1163.66906	27.92304	-1135.74602	-1021.75368
8	H	-4.9340	28.23600	358.93985	-0.01484	358.92500	387.16100
9	C	4.0180	116.80867	-1162.22279	28.21533	-1134.00745	-1017.19879
10	H	-4.9380	28.04767	359.23084	-0.09804	359.13281	387.18047
11	C	4.0297	116.15533	-1165.59742	28.13680	-1137.46062	-1021.30529
12	H	-4.9150	27.96733	357.55763	-0.45774	357.09989	385.06722
13	C	4.0197	116.37967	-1162.70488	27.89372	-1134.81116	-1018.43149
14	H	-4.9387	27.95100	359.27934	-0.10573	359.17361	387.12461
15	C	4.0233	117.88100	-1163.76548	27.92715	-1135.83832	-1017.95732

16	H	-4.9383	27.98167	359.25509	-0.15267	359.10242	387.08408
17	C	4.0277	117.30867	-1165.01891	27.96020	-1137.05871	-1019.75004
18	H	-4.9203	28.04533	357.94562	-0.38919	357.55643	385.60177
19	C	4.0150	116.23933	-1161.35502	28.02129	-1133.33374	-1017.09440
20	C	4.0570	118.91400	-1173.50370	28.52071	-1144.98299	-1026.06899
21	H	-4.9403	28.00200	359.40059	0.16847	359.56906	387.57106
	C Average	4.0284	116.64703	-1165.23103	28.06491	-1137.16612	-1020.51909
	H Average	-4.9309	28.05523	358.71675	-0.18759	358.52916	386.58439

=====

3NiCp2-STO-PBE0-TZ2P-TZ2P

Temperature: 298

Spin: 1

atensor 1 Ni

98.903 0.001 0.002
0.001 98.923 0.009
0.002 0.009 1.172
-41.212 0.000 -0.003
0.000 -41.206 -0.003
-0.003 -0.003 -2.825

atensor 2 H

-7.079 -2.511 -1.054
-2.511 -0.908 2.963
-1.054 2.963 -3.646
-0.132 -0.063 -0.076
-0.063 0.023 0.214
-0.009 0.024 0.010

atensor 3 C

1.317 -0.333 -0.997
-0.333 2.136 2.799
-0.997 2.799 12.982
-0.285 -0.034 -0.063
-0.034 -0.202 0.178
-0.006 0.017 -0.010

atensor 4 H

-0.022 0.218 -3.144
0.218 -7.971 -0.086
-3.144 -0.086 -3.648
0.045 0.005 -0.227
0.005 -0.154 -0.006
-0.026 -0.001 0.010

atensor 5 C

2.267 0.028 -2.972
0.028 1.215 -0.081
-2.972 -0.081 13.016
-0.190 0.003 -0.189
0.003 -0.297 -0.005
-0.018 -0.001 -0.010

atensor 6 H

-7.335 2.158 -0.890
2.158 -0.651 -3.017
-0.890 -3.017 -3.647
-0.139 0.054 -0.064
0.054 0.030 -0.218
-0.007 -0.025 0.010

atensor 7 C

1.284 0.286 -0.841
0.286 2.171 -2.850

-0.841 -2.850 12.980
-0.289 0.029 -0.053
0.029 -0.198 -0.181
-0.005 -0.017 -0.010

atensor 8 H
-2.556 -3.710 2.595
-3.710 -5.426 -1.779
2.595 -1.779 -3.644
-0.018 -0.093 0.188
-0.093 -0.091 -0.129
0.021 -0.015 0.010

atensor 9 C
1.921 -0.492 2.451
-0.492 1.541 -1.680
2.451 -1.681 12.981
-0.224 -0.050 0.156
-0.050 -0.263 -0.107
0.015 -0.010 -0.010

atensor 10 H
-2.975 3.846 2.493
3.846 -5.016 1.918
2.494 1.918 -3.647
-0.029 0.097 0.180
0.097 -0.080 0.139
0.020 0.016 0.010

atensor 11 C
1.872 0.510 2.356
0.510 1.601 1.812
2.356 1.812 12.995
-0.230 0.052 0.150
0.052 -0.257 0.115
0.014 0.011 -0.010

atensor 12 H
-7.331 2.157 0.890
2.157 -0.650 3.017
0.890 3.018 -3.643
-0.139 0.054 0.064
0.054 0.030 0.218
0.007 0.025 0.010

atensor 13 C
1.282 0.286 0.841
0.286 2.169 2.847
0.841 2.847 12.969
-0.289 0.029 0.054
0.029 -0.198 0.181
0.005 0.017 -0.010

atensor 14 H
-2.560 -3.711 -2.595
-3.711 -5.430 1.778
-2.595 1.778 -3.646
-0.018 -0.093 -0.188
-0.093 -0.091 0.128
-0.021 0.014 0.010

atensor 15 C
1.924 -0.491 -2.450
-0.491 1.544 1.678
-2.450 1.678 12.999
-0.224 -0.050 -0.156
-0.050 -0.263 0.107

-0.015 0.010 -0.010

atensor 16 H

-2.975 3.846 -2.493
3.846 -5.015 -1.918
-2.493 -1.918 -3.647
-0.029 0.097 -0.180
0.097 -0.080 -0.139
-0.020 -0.016 0.010

atensor 17 C

1.865 0.510 -2.354
0.510 1.597 -1.813
-2.354 -1.813 12.995
-0.230 0.052 -0.150
0.052 -0.257 -0.115
-0.014 -0.011 -0.010

atensor 18 H

-7.077 -2.511 1.054
-2.511 -0.907 -2.963
1.054 -2.963 -3.645
-0.132 -0.063 0.076
-0.063 0.023 -0.214
0.009 -0.024 0.010

atensor 19 C

1.318 -0.334 0.996
-0.334 2.135 -2.799
0.996 -2.799 12.977
-0.285 -0.034 0.063
-0.034 -0.202 -0.178
0.006 -0.017 -0.010

atensor 20 C

2.276 0.029 2.972
0.029 1.224 0.080
2.972 0.080 13.012
-0.190 0.003 0.189
0.003 -0.297 0.005
0.018 0.000 -0.010

atensor 21 H

-0.020 0.218 3.144
0.218 -7.967 0.086
3.145 0.086 -3.645
0.045 0.005 0.227
0.005 -0.154 0.006
0.026 0.001 0.010

orbtensor 1 Ni

-11669.270 -226.992 -18.012
-226.992-12421.846 -85.500
-18.012 -85.500 -161.101
2274.262 0.001 0.002
0.001 2274.257 -0.001
0.002 -0.001 2279.125

orbtensor 2 H

0.282 5.411 1.168
5.411 -12.885 -4.129
1.168 -4.129 -0.182
27.085 -4.994 -1.184
-4.994 39.358 3.327
-1.184 3.327 25.077

orbtensor 3 C

-174.266	12.389	10.346
12.389	-210.402	-24.116
10.346	-24.116	-67.754
250.533	2.301	-2.244
2.301	244.891	6.301
-2.244	6.301	232.983

orbtensor 4 H

-14.918	-0.386	3.953
-0.386	2.193	0.035
3.953	0.035	-0.129
41.123	0.434	-3.530
0.434	25.322	-0.097
-3.530	-0.097	25.076

orbtensor 5 C

-216.248	-1.162	22.659
-1.162	-165.724	2.865
22.659	2.865	-66.751
244.086	-0.200	-6.686
-0.200	251.354	-0.183
-6.686	-0.183	232.990

orbtensor 6 H

0.953	-4.541	1.415
-4.541	-13.550	4.068
1.415	4.068	-0.137
26.575	4.292	-0.999
4.292	39.867	-3.387
-0.999	-3.387	25.077

orbtensor 7 C

-175.584	-10.055	6.091
-10.055	-210.537	26.087
6.091	26.087	-66.919
250.763	-1.977	-1.895
-1.977	244.650	-6.414
-1.895	-6.414	232.981

orbtensor 8 H

-9.389	7.934	-3.116
7.934	-3.297	2.430
-3.116	2.430	-0.179
36.073	-7.380	2.912
-7.380	30.366	-1.996
2.912	-1.996	25.075

orbtensor 9 C

-198.372	23.376	-20.328
23.376	-182.800	12.641
-20.328	12.641	-66.495
246.390	3.394	5.516
3.394	249.022	-3.780
5.516	-3.780	232.985

orbtensor 10 H

-8.373	-8.237	-3.337
-8.237	-4.097	-2.521
-3.337	-2.521	-0.216
35.249	7.647	2.799
7.647	31.191	2.154
2.799	2.154	25.076

orbtensor 11 C

-195.374	-20.426	-18.863
-20.426	-186.729	-16.176
-18.863	-16.176	-67.444

246.775	-3.519	5.300
-3.519	248.640	4.080
5.300	4.080	232.985

orbtensor 12 H

0.780	-4.570	-1.190
-4.570	-13.729	-3.825
-1.190	-3.825	-0.198
26.575	4.291	0.998
4.291	39.867	3.389
0.998	3.389	25.077

orbtensor 13 C

-173.555	-9.594	-5.609
-9.594	-214.322	-23.315
-5.609	-23.315	-70.882
250.760	-1.979	1.887
-1.979	244.648	6.418
1.887	6.418	232.981

orbtensor 14 H

-9.211	7.936	3.297
7.936	-3.072	-2.309
3.297	-2.309	-0.153
36.074	-7.378	-2.915
-7.378	30.367	1.997
-2.915	1.997	25.076

orbtensor 15 C

-195.861	21.437	20.349
21.437	-185.474	-14.887
20.349	-14.887	-71.476
246.399	3.397	-5.520
3.397	249.026	3.779
-5.520	3.779	232.985

orbtensor 16 H

-8.493	-8.217	3.189
-8.217	-4.287	2.560
3.189	2.560	0.133
35.250	7.647	-2.800
7.647	31.196	-2.153
-2.800	-2.153	25.078

orbtensor 17 C

-194.524	-23.600	18.941
-23.600	-187.524	16.910
18.941	16.910	-71.772
246.781	-3.517	-5.304
-3.517	248.655	-4.075
-5.304	-4.075	232.985

orbtensor 18 H

0.390	5.372	-1.253
5.372	-12.916	3.859
-1.253	3.859	0.235
27.086	-4.995	1.181
-4.995	39.358	-3.326
1.181	-3.326	25.076

orbtensor 19 C

-175.919	11.617	-7.436
11.617	-208.819	23.279
-7.436	23.279	-72.057
250.536	2.298	2.234
2.298	244.888	-6.302
2.234	-6.302	232.981

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orbtensor 20 C
-213.786   -0.308   -25.937
-0.308  -165.347   -2.143
-25.937   -2.143  -72.543
244.076   -0.197    6.685
-0.197   251.346    0.183
6.685     0.183   232.989

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orbtensor 21 H
-14.758   -0.443   -4.111
-0.443    2.219    0.003
-4.111    0.003    0.039
41.121    0.434    3.530
0.434    25.320    0.097
3.530     0.097   25.075

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```

gtensor (ppt)
-0.094    0.000    0.000
0.000   -0.094    0.000
0.000    0.000   -0.230
87.787    2.107    0.171
2.107   94.848    0.795
0.171    0.795   -1.047

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averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	37.9183	-5808.19100	30837.53961	481.07019	31318.60980	25510.41880
2	H	-3.9107	26.24500	284.69855	0.11052	284.80907	311.05407
3	C	5.3127	91.99500	-1537.81450	32.86557	-1504.94893	-1412.95393
4	H	-3.9133	26.22233	284.89269	0.64183	285.53451	311.75685
5	C	5.3337	93.23567	-1543.89320	33.43811	-1510.45509	-1417.21942
6	H	-3.9107	26.26167	284.69855	-0.03406	284.66450	310.92616
7	C	5.3127	91.78467	-1537.81450	33.14211	-1504.67239	-1412.88772
8	H	-3.9083	26.21633	284.52868	0.63307	285.16176	311.37809
9	C	5.3153	93.57667	-1538.58640	33.39005	-1505.19635	-1411.61968
10	H	-3.9123	26.27667	284.81989	0.14328	284.96316	311.23983
11	C	5.3237	92.95100	-1540.99858	32.90975	-1508.08883	-1415.13783
12	H	-3.9077	26.12400	284.48015	-0.15767	284.32248	310.44648
13	C	5.3077	89.87667	-1536.36719	32.64986	-1503.71733	-1413.84066
14	H	-3.9117	26.36033	284.77135	0.58709	285.35844	311.71877
15	C	5.3233	91.86633	-1540.90209	33.25577	-1507.64633	-1415.77999
16	H	-3.9120	26.29233	284.79562	0.23839	285.03401	311.32635
17	C	5.3200	91.53367	-1539.93722	33.28207	-1506.65515	-1415.12148
18	H	-3.9093	26.40967	284.60148	0.21668	284.81816	311.22783
19	C	5.3110	90.53667	-1537.33206	33.24955	-1504.08252	-1413.54585
20	C	5.3383	92.24500	-1545.24402	33.28963	-1511.95439	-1419.70939
21	H	-3.9103	26.33867	284.67429	0.61208	285.28636	311.62503
	C Average	5.3198	91.96013	-1539.88898	33.14725	-1506.74173	-1414.78160
	H Average	-3.9106	26.27470	284.69613	0.29912	284.99525	311.26995

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3NiCp2-STO-PBE0-TZ2P-QZ4P
Temperature: 298
Spin: 1

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atensor 1 Ni
99.553 0.001 0.002

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0.001 99.576 0.007
0.002 0.007 1.925
-40.649 0.000 -0.003
0.000 -40.644 -0.002
-0.003 -0.002 -2.848

atensor 2 H
-6.803 -2.494 -1.052
-2.494 -0.674 2.958
-1.052 2.958 -3.463
-0.131 -0.061 -0.074
-0.061 0.019 0.209
-0.008 0.024 0.010

atensor 3 C
0.911 -0.337 -1.014
-0.337 1.739 2.846
-1.014 2.847 12.957
-0.289 -0.032 -0.063
-0.032 -0.210 0.176
-0.006 0.017 -0.011

atensor 4 H
0.208 0.217 -3.138
0.217 -7.688 -0.086
-3.139 -0.086 -3.462
0.041 0.005 -0.222
0.005 -0.153 -0.006
-0.025 -0.001 0.010

atensor 5 C
1.872 0.029 -3.024
0.029 0.806 -0.082
-3.024 -0.082 12.990
-0.199 0.003 -0.187
0.003 -0.300 -0.005
-0.018 -0.001 -0.011

atensor 6 H
-7.059 2.143 -0.888
2.143 -0.420 -3.012
-0.888 -3.012 -3.464
-0.138 0.053 -0.063
0.053 0.026 -0.213
-0.007 -0.024 0.010

atensor 7 C
0.880 0.289 -0.855
0.289 1.779 -2.899
-0.855 -2.899 12.958
-0.292 0.028 -0.053
0.028 -0.207 -0.180
-0.005 -0.017 -0.011

atensor 8 H
-2.310 -3.685 2.591
-3.685 -5.160 -1.776
2.591 -1.776 -3.458
-0.021 -0.091 0.183
-0.091 -0.091 -0.126
0.021 -0.014 0.010

atensor 9 C
1.526 -0.498 2.494
-0.498 1.141 -1.709
2.494 -1.709 12.958
-0.231 -0.048 0.154

-0.048 -0.268 -0.106
0.015 -0.010 -0.011

atensor 10 H
-2.725 3.820 2.489
3.820 -4.753 1.915
2.490 1.915 -3.462
-0.031 0.094 0.176
0.094 -0.081 0.135
0.020 0.015 0.010

atensor 11 C
1.473 0.516 2.396
0.516 1.199 1.843
2.396 1.843 12.970
-0.236 0.049 0.148
0.049 -0.262 0.114
0.014 0.011 -0.011

atensor 12 H
-7.055 2.143 0.888
2.143 -0.419 3.012
0.888 3.013 -3.461
-0.138 0.053 0.063
0.053 0.026 0.213
0.007 0.024 0.010

atensor 13 C
0.880 0.290 0.856
0.290 1.778 2.896
0.856 2.897 12.949
-0.292 0.028 0.053
0.028 -0.207 0.180
0.005 0.017 -0.011

atensor 14 H
-2.314 -3.686 -2.590
-3.686 -5.165 1.775
-2.591 1.775 -3.461
-0.021 -0.091 -0.183
-0.091 -0.091 0.125
-0.021 0.014 0.010

atensor 15 C
1.526 -0.498 -2.493
-0.498 1.141 1.707
-2.493 1.707 12.975
-0.231 -0.047 -0.154
-0.047 -0.268 0.106
-0.015 0.010 -0.011

atensor 16 H
-2.727 3.820 -2.488
3.820 -4.754 -1.915
-2.488 -1.915 -3.463
-0.031 0.094 -0.176
0.094 -0.081 -0.135
-0.020 -0.015 0.010

atensor 17 C
1.472 0.516 -2.394
0.516 1.198 -1.844
-2.395 -1.844 12.976
-0.236 0.049 -0.148
0.049 -0.262 -0.114
-0.014 -0.011 -0.011

atensor 18 H
-6.802 -2.495 1.052
-2.495 -0.673 -2.958
1.052 -2.958 -3.462
-0.132 -0.061 0.074
-0.061 0.020 -0.209
0.008 -0.024 0.010

atensor 19 C
0.910 -0.338 1.014
-0.338 1.740 -2.847
1.014 -2.847 12.953
-0.289 -0.032 0.063
-0.032 -0.210 -0.176
0.006 -0.017 -0.011

atensor 20 C
1.875 0.029 3.023
0.029 0.809 0.081
3.023 0.081 12.979
-0.199 0.003 0.187
0.003 -0.300 0.005
0.018 0.000 -0.011

atensor 21 H
0.210 0.216 3.139
0.216 -7.682 0.085
3.140 0.085 -3.458
0.041 0.005 0.222
0.005 -0.153 0.006
0.025 0.001 0.010

orbtensor 1 Ni
-11579.736 -380.054 41.363
-380.054 -11223.395 -82.255
41.363 -82.255 -579.108
2256.411 0.001 0.004
0.001 2256.404 -0.002
0.004 -0.002 2281.811

orbtensor 2 H
3.145 7.012 1.052
7.012 -14.045 -2.889
1.052 -2.889 1.353
23.908 -6.614 -0.884
-6.614 40.158 2.484
-0.884 2.484 22.986

orbtensor 3 C
-180.371 21.371 9.414
21.371 -225.874 -23.201
9.414 -23.201 -69.663
251.594 -0.518 -1.558
-0.518 252.871 4.376
-1.558 4.376 231.646

orbtensor 4 H
-16.604 -0.690 3.157
-0.690 5.805 0.126
3.157 0.126 1.426
42.496 0.575 -2.635
0.575 21.573 -0.072
-2.635 -0.072 22.985

orbtensor 5 C
-234.171 -2.112 22.455
-2.112 -182.034 1.501

22.455	1.501	-68.424
253.062	0.047	-4.644
0.047	251.418	-0.126
-4.644	-0.126	231.651

orbtensor 6 H

3.770	-5.992	0.938
-5.992	-14.815	2.940
0.938	2.940	1.512
23.233	5.683	-0.746
5.683	40.834	-2.527
-0.746	-2.527	22.986

orbtensor 7 C

-178.276	-17.184	8.350
-17.184	-229.215	23.697
8.350	23.697	-69.445
251.540	0.445	-1.314
0.445	252.923	-4.454
-1.314	-4.454	231.645

orbtensor 8 H

-9.322	10.372	-2.569
10.372	-1.187	1.742
-2.569	1.742	1.472
35.812	-9.771	2.174
-9.771	28.254	-1.490
2.174	-1.490	22.986

orbtensor 9 C

-217.619	24.258	-20.950
24.258	-192.418	11.398
-20.950	11.398	-68.953
252.529	-0.767	3.830
-0.767	251.937	-2.625
3.830	-2.625	231.649

orbtensor 10 H

-8.394	-10.785	-2.538
-10.785	-2.714	-1.806
-2.538	-1.806	1.372
34.719	10.126	2.089
10.126	29.348	1.608
2.089	1.608	22.986

orbtensor 11 C

-217.364	-26.868	-19.558
-26.868	-197.232	-13.339
-19.558	-13.339	-68.873
252.439	0.795	3.679
0.795	252.022	2.835
3.679	2.835	231.647

orbtensor 12 H

4.068	-5.930	-1.004
-5.930	-14.369	-3.330
-1.004	-3.330	1.564
23.234	5.684	0.746
5.684	40.834	2.530
0.746	2.530	22.987

orbtensor 13 C

-181.567	-17.422	-7.301
-17.422	-222.586	-22.979
-7.301	-22.979	-74.658
251.540	0.446	1.309
0.446	252.921	4.457

```

1.309      4.457      231.646

orbtensor 14 H
-9.396     10.365      2.854
10.365     -1.284      -1.757
2.854      -1.757      1.598
35.812     -9.770      -2.177
-9.770     28.255      1.492
-2.177     1.492       22.986

orbtensor 15 C
-219.010   27.712      19.224
27.712    -189.965    -14.180
19.224    -14.180    -75.050
252.529   -0.766     -3.835
-0.766    251.940     2.626
-3.835     2.626     231.649

orbtensor 16 H
-8.227    -10.777     2.766
-10.777   -2.291     2.338
2.766     2.338     1.710
34.720    10.126    -2.090
10.126    29.349    -1.608
-2.090    -1.608     22.985

orbtensor 17 C
-216.344  -24.222     19.961
-24.222  -197.930    16.076
19.961   16.076   -75.106
252.442   0.794    -3.685
0.794    252.023   -2.831
-3.685   -2.831    231.644

orbtensor 18 H
3.201     7.071     -1.121
7.071    -13.785     3.134
-1.121     3.134     1.733
23.908    -6.613     0.882
-6.613    40.160    -2.483
0.882     -2.483     22.985

orbtensor 19 C
-178.602  19.963     -6.074
19.963  -226.758    21.457
-6.074   21.457   -74.364
251.592  -0.517     1.551
-0.517   252.876   -4.376
1.551    -4.376    231.647

orbtensor 20 C
-236.077  -4.640    -26.280
-4.640  -179.097   -0.122
-26.280  -0.122  -75.385
253.064   0.043    4.642
0.043   251.418    0.127
4.642    0.127    231.655

orbtensor 21 H
-16.562   -0.656    -3.429
-0.656    5.854    -0.320
-3.429   -0.320    1.664
42.496    0.574    2.635
0.574    21.573    0.072
2.635    0.072    22.985

gtensor (ppt)

```

```

-0.114    0.000    0.000
0.000   -0.114    0.000
0.000    0.000   -0.236
86.727    3.556   -0.382
3.556   83.338    0.766
-0.382    0.766    2.905

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	38.9710	-5529.20433	31649.25914	431.22887	32080.48801	26551.28367
2	H	-3.6807	25.83500	267.57927	0.49401	268.07328	293.90828
3	C	5.0323	86.73433	-1454.62920	30.39318	-1424.23602	-1337.50169
4	H	-3.6813	25.89367	267.62774	0.01435	267.64209	293.53576
5	C	5.0527	83.83400	-1460.50669	30.28685	-1430.21984	-1346.38584
6	H	-3.6817	25.84000	267.65197	0.22030	267.87227	293.71227
7	C	5.0357	86.39067	-1455.59273	30.59368	-1424.99905	-1338.60838
8	H	-3.6767	26.00500	267.28848	0.53647	267.82494	293.82994
9	C	5.0383	85.70833	-1456.36354	30.79464	-1425.56891	-1339.86057
10	H	-3.6807	25.77233	267.57927	-0.16025	267.41902	293.19135
11	C	5.0443	84.21300	-1458.09788	30.19098	-1427.90690	-1343.69390
12	H	-3.6790	26.10600	267.45811	0.12430	267.58241	293.68841
13	C	5.0323	85.76533	-1454.62920	30.20525	-1424.42396	-1338.65862
14	H	-3.6807	25.99033	267.57927	0.42258	268.00185	293.99218
15	C	5.0440	84.03100	-1458.00153	30.40053	-1427.60100	-1343.57000
16	H	-3.6820	26.08200	267.67620	-0.13468	267.54152	293.62352
17	C	5.0457	82.24300	-1458.48329	30.30512	-1428.17817	-1345.93517
18	H	-3.6797	26.06733	267.50657	0.62460	268.13118	294.19851
19	C	5.0310	85.46367	-1454.24379	30.88019	-1423.36360	-1337.89993
20	C	5.0510	81.85933	-1460.02493	30.46230	-1429.56263	-1347.70330
21	H	-3.6773	26.00333	267.33694	0.06996	267.40690	293.41023
C Average		5.0407	84.62427	-1457.05728	30.45127	-1426.60601	-1341.98174
H Average		-3.6800	25.95950	267.52838	0.22116	267.74955	293.70905

3NiCp2-STO-PBE0-QZ4P-DZ

Temperature: 298

Spin: 1

atensor 1 Ni

```

120.794 0.015 0.006
0.015 120.733 0.010
0.006 0.010 17.277
-43.908 -0.005 -0.004
-0.005 -43.885 -0.003
-0.004 -0.003 -2.755

```

atensor 2 H

```

-7.696 -2.556 -1.052
-2.556 -1.409 2.951
-1.052 2.951 -4.906
-0.152 -0.075 -0.085
-0.075 0.032 0.240
-0.009 0.026 0.007

```

atensor 3 C

```

0.270 -0.377 -0.966
-0.377 1.198 2.671
-0.966 2.671 11.375

```


-0.281 -0.032 -0.066
-0.033 -0.199 0.186
-0.008 0.021 -0.009

atensor 4 H
-0.519 0.222 -3.131
0.222 -8.628 -0.086
-3.131 -0.086 -4.928
0.059 0.006 -0.254
0.006 -0.178 -0.007
-0.028 -0.001 0.007

atensor 5 C
1.354 0.033 -2.851
0.033 0.162 -0.079
-2.851 -0.079 11.448
-0.188 0.003 -0.197
0.003 -0.293 -0.005
-0.022 -0.001 -0.009

atensor 6 H
-7.956 2.197 -0.888
2.197 -1.144 -3.004
-0.888 -3.005 -4.903
-0.159 0.064 -0.072
0.064 0.040 -0.244
-0.008 -0.027 0.007

atensor 7 C
0.237 0.325 -0.817
0.325 1.240 -2.722
-0.817 -2.722 11.385
-0.285 0.028 -0.056
0.028 -0.196 -0.189
-0.006 -0.021 -0.009

atensor 8 H
-3.106 -3.774 2.583
-3.774 -6.024 -1.772
2.583 -1.772 -4.921
-0.017 -0.111 0.210
-0.111 -0.102 -0.144
0.023 -0.016 0.007

atensor 9 C
0.964 -0.555 2.334
-0.555 0.534 -1.609
2.334 -1.609 11.346
-0.220 -0.049 0.163
-0.048 -0.259 -0.112
0.018 -0.012 -0.009

atensor 10 H
-3.529 3.913 2.482
3.913 -5.605 1.911
2.482 1.911 -4.924
-0.029 0.115 0.202
0.115 -0.090 0.155
0.022 0.017 0.007

atensor 11 C
0.911 0.574 2.243
0.574 0.605 1.733
2.243 1.733 11.363
-0.226 0.051 0.157
0.050 -0.253 0.120
0.017 0.013 -0.009

atensor 12 H
-7.951 2.196 0.888
2.196 -1.142 3.005
0.888 3.005 -4.899
-0.159 0.064 0.072
0.064 0.040 0.244
0.008 0.027 0.007

atensor 13 C
0.236 0.325 0.818
0.325 1.239 2.720
0.818 2.720 11.377
-0.285 0.028 0.056
0.028 -0.196 0.189
0.006 0.021 -0.009

atensor 14 H
-3.109 -3.775 -2.583
-3.775 -6.029 1.772
-2.583 1.772 -4.924
-0.017 -0.111 -0.210
-0.110 -0.102 0.144
-0.023 0.016 0.007

atensor 15 C
0.965 -0.554 -2.332
-0.554 0.535 1.607
-2.332 1.607 11.359
-0.220 -0.049 -0.163
-0.048 -0.259 0.112
-0.018 0.012 -0.009

atensor 16 H
-3.530 3.913 -2.481
3.913 -5.605 -1.910
-2.482 -1.910 -4.925
-0.029 0.115 -0.202
0.114 -0.090 -0.155
-0.022 -0.017 0.007

atensor 17 C
0.905 0.574 -2.242
0.574 0.601 -1.733
-2.242 -1.733 11.365
-0.226 0.051 -0.156
0.050 -0.253 -0.120
-0.017 -0.013 -0.009

atensor 18 H
-7.694 -2.556 1.051
-2.556 -1.408 -2.951
1.051 -2.951 -4.905
-0.152 -0.075 0.085
-0.075 0.032 -0.240
0.009 -0.026 0.007

atensor 19 C
0.270 -0.378 0.965
-0.378 1.197 -2.671
0.965 -2.671 11.370
-0.281 -0.032 0.066
-0.033 -0.199 -0.186
0.008 -0.021 -0.009

atensor 20 C
1.360 0.033 2.851

0.033 0.168 0.078
2.851 0.078 11.445
-0.188 0.003 0.198
0.003 -0.294 0.005
0.022 0.001 -0.009

atensor 21 H
-0.517 0.222 3.131
0.222 -8.625 0.086
3.132 0.086 -4.925
0.059 0.006 0.254
0.006 -0.178 0.007
0.028 0.001 0.007

orbtensor 1 Ni
-11147.403 369.343 -17.403
369.343-11375.163 3.096
-17.403 3.096 -167.137
2268.396 -0.002 0.003
-0.002 2268.405 0.000
0.003 0.000 2278.779

orbtensor 2 H
3.083 4.046 0.540
4.046 -6.850 -0.953
0.540 -0.953 2.733
24.812 -4.458 -0.296
-4.458 35.774 0.834
-0.296 0.834 24.265

orbtensor 3 C
-147.658 14.044 9.351
14.044 -171.351 -18.796
9.351 -18.796 -54.090
249.771 7.716 -0.916
7.716 230.955 2.615
-0.916 2.615 239.310

orbtensor 4 H
-8.362 -0.452 0.977
-0.452 4.837 -0.083
0.977 -0.083 2.820
37.323 0.387 -0.890
0.387 23.215 -0.024
-0.890 -0.024 24.249

orbtensor 5 C
-181.936 -0.032 19.020
-0.032 -149.453 -1.152
19.020 -1.152 -52.503
228.120 -0.677 -2.744
-0.677 252.542 -0.070
-2.744 -0.070 239.327

orbtensor 6 H
3.593 -3.691 0.082
-3.691 -7.226 0.983
0.082 0.983 2.841
24.347 3.831 -0.250
3.831 36.224 -0.851
-0.250 -0.851 24.257

orbtensor 7 C
-144.871 -13.316 7.679
-13.316 -174.427 18.885
7.679 18.885 -55.358
250.544 -6.648 -0.767

-6.648 230.149 -2.661
-0.767 -2.661 239.294

orbtensor 8 H
-4.479 6.084 -0.913
6.084 0.591 0.663
-0.913 0.663 2.793
32.834 -6.582 0.720
-6.582 27.743 -0.495
0.720 -0.495 24.265

orbtensor 9 C
-177.389 14.049 -18.097
14.049 -154.657 9.558
-18.097 9.558 -52.902
235.960 11.351 2.275
11.351 244.738 -1.561
2.275 -1.561 239.285

orbtensor 10 H
-3.560 -6.433 -0.668
-6.433 0.010 -0.503
-0.668 -0.503 2.715
32.087 6.820 0.690
6.820 28.470 0.532
0.690 0.532 24.253

orbtensor 11 C
-174.001 -16.692 -17.252
-16.692 -154.200 -8.725
-17.252 -8.725 -53.929
237.215 -11.773 2.180
-11.773 243.466 1.679
2.180 1.679 239.266

orbtensor 12 H
3.391 -3.657 -0.181
-3.657 -7.298 -1.149
-0.181 -1.149 2.872
24.347 3.831 0.250
3.831 36.225 0.852
0.250 0.852 24.258

orbtensor 13 C
-145.389 -14.455 -8.009
-14.455 -177.542 -20.222
-8.009 -20.222 -53.982
250.544 -6.649 0.762
-6.649 230.149 2.660
0.762 2.660 239.296

orbtensor 14 H
-4.437 6.132 0.723
6.132 0.778 -0.633
0.723 -0.633 2.810
32.835 -6.582 -0.722
-6.582 27.745 0.496
-0.722 0.496 24.265

orbtensor 15 C
-174.225 13.358 15.569
13.358 -153.264 -9.669
15.569 -9.669 -54.750
235.968 11.352 -2.274
11.352 244.745 1.557
-2.274 1.557 239.284

```

orbtensor 16 H
-3.701  -6.347   0.627
-6.347   0.035   0.664
0.627   0.664   2.729
32.089   6.820  -0.692
6.820  28.471  -0.533
-0.692  -0.533  24.253

```

```

orbtensor 17 C
-173.293 -17.726  16.408
-17.726 -155.541  10.983
16.408  10.983 -52.839
237.224 -11.774  -2.181
-11.774 243.471  -1.677
-2.181  -1.677 239.260

```

```

orbtensor 18 H
2.994  4.134  -0.401
4.134 -6.844  1.072
-0.401 1.072  2.712
24.812 -4.457  0.295
-4.457 35.775 -0.833
0.295 -0.833 24.266

```

```

orbtensor 19 C
-147.078 13.534  -5.802
13.534 -173.563  20.460
-5.802  20.460 -52.864
249.766  7.723  0.912
7.723 230.954  -2.615
0.912  -2.615 239.303

```

```

orbtensor 20 C
-181.778 -0.931  -18.180
-0.931 -150.027  -1.441
-18.180 -1.441  -54.394
228.119 -0.680  2.745
-0.680 252.541  0.070
2.745  0.070 239.335

```

```

orbtensor 21 H
-8.444  -0.373  -0.842
-0.373   5.052  -0.039
-0.842  -0.039  2.784
37.323   0.386   0.891
0.386  23.216   0.024
0.891   0.024  24.251

```

```

gtensor (ppt)
-0.092  0.000  0.000
0.000 -0.092  0.000
0.000  0.000 -0.233
83.760 -3.487  0.168
-3.487 85.831 -0.030
0.168 -0.030 -0.985

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	56.0853	-5291.37433	45516.38872	469.32121	45985.70993	40694.33559
2	H	-4.7080	27.93900	342.02585	-0.48124	341.54460	369.48360

3	C	4.1180	115.64567	-1189.50354	28.97182	-1160.53172	-1044.88605
4	H	-4.7290	28.02733	343.55145	-0.06083	343.49062	371.51795
5	C	4.1580	112.03233	-1201.05773	29.38428	-1171.67344	-1059.64111
6	H	-4.7050	28.01200	341.80790	-0.09152	341.71638	369.72838
7	C	4.1240	115.11033	-1191.23667	29.21451	-1162.02215	-1046.91182
8	H	-4.7210	27.91567	342.97027	-0.48923	342.48103	370.39670
9	C	4.1187	111.67833	-1189.69611	28.79459	-1160.90152	-1049.22318
10	H	-4.7233	27.99167	343.13978	0.15191	343.29168	371.28335
11	C	4.1303	112.60567	-1193.06608	29.22127	-1163.84481	-1051.23914
12	H	-4.7013	27.93167	341.54153	-0.09413	341.44740	369.37906
13	C	4.1207	114.35867	-1190.27382	29.18495	-1161.08887	-1046.73020
14	H	-4.7247	27.99867	343.23664	-0.46462	342.77202	370.77069
15	C	4.1237	112.58600	-1191.14038	28.91263	-1162.22775	-1049.64175
16	H	-4.7240	27.95867	343.18821	0.16920	343.35741	371.31608
17	C	4.1277	112.76067	-1192.29580	29.30304	-1162.99276	-1050.23209
18	H	-4.7067	27.90500	341.92898	-0.49460	341.43438	369.33938
19	C	4.1160	115.50600	-1188.92583	28.91240	-1160.01343	-1044.50743
20	C	4.1607	111.26533	-1201.82800	29.26894	-1172.55906	-1061.29373
21	H	-4.7263	28.06067	343.35772	-0.08625	343.27147	371.33214
C Average		4.1298	113.35490	-1192.90239	29.11684	-1163.78555	-1050.43065
H Average		-4.7169	27.97403	342.67483	-0.19413	342.48070	370.45473

=====
3NiCp2-STO-PBE0-QZ4P-TZ2P
Temperature: 298
Spin: 1

atensor 1 Ni
122.616 -0.001 0.006
-0.001 122.638 0.009
0.006 0.009 18.459
-44.651 0.000 -0.004
0.000 -44.645 -0.003
-0.004 -0.003 -2.647

atensor 2 H
-7.062 -2.510 -1.054
-2.510 -0.895 2.962
-1.054 2.962 -3.627
-0.140 -0.067 -0.080
-0.067 0.024 0.225
-0.009 0.025 0.010

atensor 3 C
1.322 -0.336 -0.997
-0.336 2.149 2.798
-0.997 2.799 12.968
-0.300 -0.035 -0.067
-0.035 -0.214 0.188
-0.007 0.019 -0.011

atensor 4 H
-0.009 0.218 -3.142
0.218 -7.952 -0.086
-3.143 -0.086 -3.628
0.048 0.006 -0.239
0.006 -0.163 -0.007
-0.027 -0.001 0.010

atensor 5 C
2.284 0.029 -2.972
0.029 1.220 -0.081
-2.972 -0.081 13.002
-0.202 0.003 -0.199
0.003 -0.313 -0.005

-0.020 -0.001 -0.011

atensor 6 H

-7.318 2.156 -0.889
2.156 -0.638 -3.016
-0.889 -3.016 -3.627
-0.147 0.057 -0.068
0.057 0.031 -0.229
-0.008 -0.026 0.010

atensor 7 C

1.289 0.289 -0.841
0.289 2.184 -2.849
-0.841 -2.849 12.965
-0.304 0.030 -0.056
0.030 -0.211 -0.191
-0.006 -0.019 -0.011

atensor 8 H

-2.542 -3.707 2.594
-3.707 -5.410 -1.778
2.594 -1.778 -3.625
-0.020 -0.099 0.197
-0.098 -0.096 -0.135
0.022 -0.015 0.010

atensor 9 C

1.932 -0.497 2.451
-0.497 1.549 -1.680
2.451 -1.680 12.968
-0.237 -0.052 0.164
-0.052 -0.277 -0.113
0.016 -0.011 -0.011

atensor 10 H

-2.959 3.843 2.492
3.843 -4.999 1.917
2.493 1.917 -3.627
-0.031 0.102 0.189
0.102 -0.085 0.146
0.021 0.016 0.010

atensor 11 C

1.884 0.515 2.356
0.515 1.610 1.812
2.356 1.812 12.980
-0.243 0.054 0.158
0.054 -0.271 0.121
0.016 0.012 -0.011

atensor 12 H

-7.313 2.156 0.889
2.156 -0.637 3.016
0.890 3.017 -3.623
-0.147 0.057 0.068
0.057 0.031 0.229
0.008 0.026 0.010

atensor 13 C

1.287 0.289 0.841
0.289 2.182 2.847
0.841 2.847 12.954
-0.304 0.030 0.056
0.030 -0.211 0.191
0.006 0.019 -0.011

atensor 14 H

-2.546 -3.708 -2.594
-3.708 -5.414 1.777
-2.594 1.778 -3.627
-0.020 -0.098 -0.197
-0.098 -0.096 0.135
-0.022 0.015 0.010

atensor 15 C
1.936 -0.496 -2.450
-0.496 1.552 1.678
-2.450 1.678 12.984
-0.237 -0.052 -0.164
-0.052 -0.277 0.113
-0.016 0.011 -0.011

atensor 16 H
-2.960 3.843 -2.492
3.843 -4.999 -1.917
-2.492 -1.917 -3.627
-0.031 0.102 -0.189
0.102 -0.085 -0.145
-0.021 -0.016 0.010

atensor 17 C
1.876 0.515 -2.354
0.515 1.605 -1.812
-2.354 -1.813 12.980
-0.243 0.054 -0.158
0.054 -0.271 -0.121
-0.016 -0.012 -0.011

atensor 18 H
-7.059 -2.510 1.053
-2.510 -0.894 -2.962
1.053 -2.962 -3.626
-0.140 -0.067 0.080
-0.067 0.024 -0.225
0.009 -0.025 0.010

atensor 19 C
1.321 -0.337 0.996
-0.337 2.147 -2.798
0.996 -2.798 12.962
-0.300 -0.035 0.067
-0.035 -0.214 -0.188
0.007 -0.019 -0.011

atensor 20 C
2.292 0.029 2.972
0.029 1.229 0.080
2.972 0.080 13.000
-0.202 0.003 0.199
0.003 -0.313 0.005
0.020 0.001 -0.011

atensor 21 H
-0.008 0.218 3.143
0.218 -7.949 0.086
3.144 0.086 -3.625
0.048 0.006 0.239
0.006 -0.163 0.007
0.027 0.001 0.010

orbtensor 1 Ni
-12618.237 287.461 7.756
287.461-12830.314 -72.283
7.756 -72.283 -643.061

2271.851	0.000	0.002
0.000	2271.854	0.000
0.002	0.000	2279.921

orbtensor 2 H

-0.401	5.474	1.325
5.474	-13.442	-3.163
1.325	-3.163	-0.293
27.572	-5.020	-0.957
-5.020	39.910	2.692
-0.957	2.692	25.221

orbtensor 3 C

-176.889	18.082	7.832
18.082	-210.725	-22.446
7.832	-22.446	-69.386
255.248	2.413	-1.528
2.413	249.332	4.289
-1.528	4.289	233.522

orbtensor 4 H

-15.453	-0.613	3.266
-0.613	1.927	0.217
3.266	0.217	-0.262
41.686	0.436	-2.855
0.436	25.800	-0.078
-2.855	-0.078	25.220

orbtensor 5 C

-220.950	0.300	20.871
0.300	-175.044	0.659
20.871	0.659	-68.192
248.493	-0.209	-4.548
-0.209	256.115	-0.124
-4.548	-0.124	233.529

orbtensor 6 H

0.231	-4.722	0.749
-4.722	-14.131	3.377
0.749	3.377	-0.169
27.060	4.315	-0.808
4.315	40.423	-2.739
-0.808	-2.739	25.221

orbtensor 7 C

-172.285	-15.881	7.188
-15.881	-215.881	22.343
7.188	22.343	-68.946
255.494	-2.073	-1.290
-2.073	249.083	-4.365
-1.290	-4.365	233.519

orbtensor 8 H

-10.189	7.958	-2.781
7.958	-3.444	1.842
-2.781	1.842	-0.180
36.609	-7.419	2.355
-7.419	30.873	-1.614
2.355	-1.614	25.219

orbtensor 9 C

-208.966	19.529	-17.806
19.529	-184.581	12.540
-17.806	12.540	-68.359
250.913	3.561	3.753
3.561	253.673	-2.571
3.753	-2.571	233.522

orbtensor 10 H
-9.137 -8.390 -2.546
-8.390 -4.590 -2.074
-2.546 -2.074 -0.223
35.782 7.688 2.263
7.688 31.703 1.741
2.263 1.741 25.221

orbtensor 11 C
-206.872 -23.927 -18.299
-23.927 -186.431 -13.282
-18.299 -13.282 -69.204
251.318 -3.691 3.605
-3.691 253.274 2.775
3.605 2.775 233.523

orbtensor 12 H
0.332 -4.594 -0.994
-4.594 -13.841 -3.719
-0.994 -3.719 -0.054
27.060 4.314 0.808
4.314 40.423 2.742
0.808 2.742 25.222

orbtensor 13 C
-173.001 -17.302 -5.875
-17.302 -211.591 -21.517
-5.875 -21.517 -73.229
255.491 -2.076 1.284
-2.076 249.080 4.369
1.284 4.369 233.519

orbtensor 14 H
-10.034 7.794 3.259
7.794 -3.470 -2.055
3.259 -2.055 0.011
36.610 -7.418 -2.358
-7.418 30.873 1.615
-2.358 1.615 25.221

orbtensor 15 C
-207.974 20.296 19.933
20.296 -180.993 -15.939
19.933 -15.939 -74.071
250.920 3.563 -3.756
3.563 253.675 2.570
-3.756 2.570 233.524

orbtensor 16 H
-8.796 -8.213 2.968
-8.213 -4.313 2.427
2.968 2.427 -0.027
35.782 7.688 -2.265
7.688 31.705 -1.741
-2.265 -1.741 25.222

orbtensor 17 C
-203.715 -20.796 17.839
-20.796 -184.107 15.529
17.839 15.529 -73.265
251.319 -3.689 -3.609
-3.689 253.284 -2.771
-3.609 -2.771 233.524

orbtensor 18 H
-0.406 5.405 -1.329

```

5.405  -13.132  3.431
-1.329   3.431  -0.068
27.573  -5.021  0.956
-5.021  39.910  -2.691
0.956   -2.691  25.220

```

```

orbtensor 19 C
-173.774  17.537  -7.228
17.537  -210.113  23.220
-7.228  23.220  -72.661
255.250  2.411  1.519
2.411  249.328  -4.290
1.519  -4.290  233.519

```

```

orbtensor 20 C
-217.362  -1.994  -24.778
-1.994  -173.568  -0.185
-24.778  -0.185  -73.202
248.485  -0.207  4.546
-0.207  256.112  0.125
4.546  0.125  233.526

```

```

orbtensor 21 H
-15.107  -0.538  -3.845
-0.538  1.914  -0.233
-3.845  -0.233  -0.080
41.685  0.436  2.854
0.436  25.800  0.078
2.854  0.078  25.220

```

```

gtensor (ppt)
-0.096  0.000  0.000
0.000  -0.096  0.000
0.000  0.000  -0.237
96.928  -2.721  -0.070
-2.721  98.865  0.684
-0.070  0.684  3.469

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	57.2567	-6422.66200	46697.58250	515.09915	47212.68165	40790.01965
2	H	-3.8967	26.18900	284.48906	0.02253	284.51159	310.70059
3	C	5.3047	93.70067	-1539.88164	33.52280	-1506.35884	-1412.65817
4	H	-3.8980	26.30600	284.58641	0.41482	285.00122	311.30722
5	C	5.3267	91.31700	-1546.26797	33.95073	-1512.31724	-1421.00024
6	H	-3.8963	26.21167	284.46473	0.42338	284.88811	311.09977
7	C	5.3040	93.66133	-1539.68811	34.06052	-1505.62759	-1411.96626
8	H	-3.8943	26.29600	284.31871	0.13495	284.45366	310.74966
9	C	5.3080	92.06733	-1540.84926	33.84385	-1507.00541	-1414.93808
10	H	-3.8970	26.25200	284.51340	0.56007	285.07346	311.32546
11	C	5.3163	91.86933	-1543.26833	33.90687	-1509.36146	-1417.49213
12	H	-3.8930	26.38067	284.22136	0.32603	284.54740	310.92806
13	C	5.2990	93.42300	-1538.23667	33.66747	-1504.56920	-1411.14620
14	H	-3.8977	26.40367	284.56207	0.06786	284.62993	311.03360
15	C	5.3157	91.69367	-1543.07480	33.62493	-1509.44988	-1417.75621
16	H	-3.8973	26.52433	284.53773	0.61617	285.15391	311.67824
17	C	5.3120	92.34667	-1542.01042	34.13436	-1507.87605	-1415.52938
18	H	-3.8950	26.36567	284.36738	0.12479	284.49217	310.85784
19	C	5.3017	93.84967	-1539.01077	33.89423	-1505.11654	-1411.26688
20	C	5.3317	91.33033	-1547.71941	33.94940	-1513.77002	-1422.43969

21	H	-3.8957	26.47733	284.41605	0.42343	284.83948	311.31682
C Average		5.3120	92.52590	-1542.00074	33.85552	-1508.14522	-1415.61932
H Average		-3.8961	26.34063	284.44769	0.31140	284.75909	311.09973

=====

3NiCp2-STO-PBE0-QZ4P-QZ4P

Temperature: 298

Spin: 1

atensor 1 Ni

123.001 -0.001 0.006
-0.001 123.025 0.006
0.006 0.006 18.628
-44.492 0.000 -0.004
0.000 -44.487 -0.003
-0.004 -0.003 -2.642

atensor 2 H

-6.772 -2.488 -1.055
-2.488 -0.658 2.966
-1.055 2.966 -3.430
-0.140 -0.066 -0.079
-0.066 0.022 0.223
-0.009 0.025 0.010

atensor 3 C

0.967 -0.340 -1.013
-0.340 1.803 2.846
-1.014 2.847 12.940
-0.305 -0.034 -0.067
-0.034 -0.220 0.187
-0.006 0.018 -0.011

atensor 4 H

0.222 0.216 -3.147
0.216 -7.654 -0.086
-3.147 -0.086 -3.429
0.045 0.006 -0.236
0.006 -0.164 -0.006
-0.026 -0.001 0.010

atensor 5 C

1.937 0.030 -3.024
0.030 0.862 -0.082
-3.024 -0.082 12.971
-0.208 0.003 -0.199
0.003 -0.317 -0.005
-0.019 -0.001 -0.011

atensor 6 H

-7.027 2.138 -0.890
2.138 -0.404 -3.020
-0.890 -3.020 -3.431
-0.147 0.057 -0.067
0.057 0.028 -0.227
-0.007 -0.025 0.010

atensor 7 C

0.936 0.292 -0.855
0.292 1.843 -2.899
-0.855 -2.899 12.939
-0.309 0.030 -0.056
0.030 -0.217 -0.191
-0.005 -0.018 -0.011

atensor 8 H
-2.290 -3.676 2.597
-3.676 -5.134 -1.781
2.598 -1.781 -3.426
-0.022 -0.098 0.195
-0.097 -0.097 -0.134
0.022 -0.015 0.010

atensor 9 C
1.588 -0.503 2.494
-0.503 1.199 -1.709
2.494 -1.709 12.942
-0.243 -0.051 0.164
-0.051 -0.282 -0.113
0.015 -0.011 -0.011

atensor 10 H
-2.704 3.810 2.496
3.810 -4.727 1.920
2.496 1.920 -3.429
-0.033 0.101 0.188
0.101 -0.086 0.144
0.021 0.016 0.010

atensor 11 C
1.534 0.521 2.396
0.521 1.258 1.843
2.396 1.843 12.951
-0.249 0.053 0.158
0.053 -0.277 0.121
0.015 0.011 -0.011

atensor 12 H
-7.024 2.138 0.891
2.138 -0.404 3.020
0.891 3.021 -3.428
-0.147 0.057 0.067
0.057 0.028 0.227
0.007 0.025 0.010

atensor 13 C
0.937 0.292 0.856
0.292 1.842 2.897
0.856 2.897 12.932
-0.309 0.030 0.056
0.030 -0.217 0.191
0.005 0.018 -0.011

atensor 14 H
-2.294 -3.677 -2.597
-3.677 -5.138 1.780
-2.597 1.780 -3.428
-0.022 -0.097 -0.195
-0.097 -0.097 0.134
-0.022 0.015 0.010

atensor 15 C
1.587 -0.502 -2.493
-0.502 1.199 1.707
-2.493 1.707 12.956
-0.243 -0.051 -0.164
-0.051 -0.282 0.112
-0.015 0.011 -0.011

atensor 16 H
-2.706 3.811 -2.495
3.811 -4.728 -1.920

-2.495 -1.920 -3.430
-0.033 0.101 -0.187
0.101 -0.086 -0.144
-0.021 -0.016 0.010

atensor 17 C
1.533 0.521 -2.394
0.521 1.257 -1.844
-2.394 -1.844 12.958
-0.249 0.053 -0.158
0.053 -0.276 -0.121
-0.015 -0.011 -0.011

atensor 18 H
-6.770 -2.488 1.055
-2.488 -0.657 -2.966
1.055 -2.966 -3.429
-0.140 -0.066 0.079
-0.066 0.022 -0.223
0.009 -0.025 0.010

atensor 19 C
0.966 -0.340 1.014
-0.340 1.803 -2.847
1.014 -2.847 12.934
-0.305 -0.034 0.067
-0.034 -0.220 -0.187
0.006 -0.018 -0.011

atensor 20 C
1.940 0.029 3.023
0.029 0.865 0.081
3.023 0.081 12.962
-0.208 0.003 0.199
0.003 -0.317 0.005
0.019 0.000 -0.011

atensor 21 H
0.223 0.216 3.148
0.216 -7.650 0.086
3.148 0.086 -3.425
0.045 0.006 0.237
0.006 -0.164 0.006
0.026 0.001 0.010

orbtensor 1 Ni
-12750.290 159.720 18.833
159.720-11977.470 17.398
18.833 17.398 8.387
2263.345 0.000 0.003
0.000 2263.346 -0.002
0.003 -0.002 2284.890

orbtensor 2 H
2.624 6.584 1.253
6.584 -13.462 -2.024
1.253 -2.024 1.307
24.694 -6.135 -0.665
-6.135 39.768 1.868
-0.665 1.868 23.092

orbtensor 3 C
-186.041 18.074 8.167
18.074 -221.737 -21.727
8.167 -21.727 -67.955
251.604 -0.037 -1.387
-0.037 251.699 3.897

```

-1.387    3.897    230.676

orbtensor 4 H
-15.806   -0.802     2.358
-0.802    4.620     0.411
2.358     0.411     1.341
41.937    0.533    -1.981
0.533    22.528    -0.054
-1.981   -0.054    23.091

orbtensor 5 C
-227.015  -2.392    20.364
-2.392  -177.854  -0.717
20.364   -0.717  -68.094
251.723   0.006   -4.133
0.006   251.603  -0.113
-4.133   -0.113  230.682

orbtensor 6 H
3.334   -5.409     0.276
-5.409  -14.206    2.242
0.276   2.242     1.336
24.066   5.272    -0.561
5.272   40.395   -1.900
-0.561  -1.900    23.092

orbtensor 7 C
-179.928  -12.888     6.957
-12.888  -225.493    21.091
6.957    21.091  -67.985
251.596   0.031   -1.171
0.031   251.701  -3.965
-1.171   -3.965  230.674

orbtensor 8 H
-9.400    9.426    -2.215
9.426   -1.734     1.049
-2.215    1.049     1.331
35.735   -9.065     1.634
-9.065   28.724    -1.120
1.634   -1.120    23.092

orbtensor 9 C
-208.452  21.997   -17.625
21.997  -187.173   10.974
-17.625  10.974   -67.710
251.672  -0.058    3.410
-0.058  251.628   -2.336
3.410   -2.336   230.678

orbtensor 10 H
-8.024   -9.784    -1.572
-9.784   -3.111    -1.573
-1.572   -1.573     1.304
34.722    9.394     1.571
9.394   29.739     1.209
1.571    1.209    23.092

orbtensor 11 C
-204.204  -25.758   -18.809
-25.758  -192.814  -10.207
-18.809  -10.207   -67.093
251.665   0.059    3.275
0.059   251.637    2.523
3.275    2.523   230.678

orbtensor 12 H

```

3.793	-5.419	-0.626
-5.419	-13.950	-2.622
-0.626	-2.622	1.684
24.067	5.272	0.561
5.272	40.395	1.903
0.561	1.903	23.093

orbtensor 13 C

-182.265	-13.128	-4.588
-13.128	-223.100	-19.419
-4.588	-19.419	-73.873
251.594	0.033	1.166
0.033	251.698	3.969
1.166	3.969	230.672

orbtensor 14 H

-9.303	9.422	2.501
9.422	-1.602	-1.434
2.501	-1.434	1.529
35.736	-9.064	-1.638
-9.064	28.725	1.122
-1.638	1.122	23.092

orbtensor 15 C

-210.014	24.928	17.835
24.928	-186.422	-12.860
17.835	-12.860	-73.485
251.675	-0.057	-3.414
-0.057	251.633	2.337
-3.414	2.337	230.679

orbtensor 16 H

-7.766	-9.901	2.032
-9.901	-2.771	1.697
2.032	1.697	1.446
34.723	9.394	-1.572
9.394	29.739	-1.209
-1.572	-1.209	23.091

orbtensor 17 C

-202.481	-25.190	18.931
-25.190	-195.521	13.621
18.931	13.621	-73.439
251.668	0.059	-3.281
0.059	251.639	-2.519
-3.281	-2.519	230.675

orbtensor 18 H

2.811	6.642	-1.145
6.642	-13.287	2.394
-1.145	2.394	1.542
24.693	-6.134	0.663
-6.134	39.770	-1.867
0.663	-1.867	23.092

orbtensor 19 C

-183.405	16.018	-8.263
16.018	-224.252	18.427
-8.263	18.427	-72.909
251.600	-0.036	1.381
-0.036	251.703	-3.897
1.381	-3.897	230.674

orbtensor 20 C

-226.589	-5.449	-23.701
-5.449	-175.356	0.965
-23.701	0.965	-73.933


```

251.724    0.002    4.131
0.002 251.598    0.113
4.131    0.113 230.683

```

```

orbtensor 21 H
-15.662   -0.770   -2.989
-0.770    4.805   -0.263
-2.989   -0.263    1.694
41.937    0.532    1.981
0.532   22.528    0.054
1.981    0.054   23.092

```

```

gtensor (ppt)
-0.092    0.000    0.000
0.000   -0.092    0.000
0.000    0.000   -0.233
97.911   -1.505   -0.174
-1.505   90.603   -0.165
-0.174   -0.165   -2.807

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Ni	57.6777	-5969.26400	46938.28485	532.59593	47470.88079	41501.61679
2	H	-3.6560	26.00767	266.33589	0.45673	266.79262	292.80029
3	C	5.0580	86.08200	-1465.07299	35.92228	-1429.15071	-1343.06871
4	H	-3.6567	25.90367	266.38446	-0.08167	266.30279	292.20645
5	C	5.0780	87.01500	-1470.86608	35.58906	-1435.27702	-1348.26202
6	H	-3.6570	26.00567	266.40874	0.62383	267.03257	293.03824
7	C	5.0603	86.85500	-1465.74885	35.92924	-1429.81961	-1342.96461
8	H	-3.6530	25.91600	266.11735	0.01580	266.13314	292.04914
9	C	5.0643	90.21433	-1466.90747	35.63294	-1431.27453	-1341.06019
10	H	-3.6563	25.90733	266.36018	0.33907	266.69925	292.60658
11	C	5.0687	89.95633	-1468.16264	35.88934	-1432.27330	-1342.31697
12	H	-3.6550	26.36067	266.26304	0.65687	266.91991	293.28058
13	C	5.0580	84.90867	-1465.07299	36.02922	-1429.04377	-1344.13510
14	H	-3.6563	26.05900	266.36018	0.00955	266.36973	292.42873
15	C	5.0687	88.02200	-1468.16264	35.64775	-1432.51489	-1344.49289
16	H	-3.6577	26.15400	266.45731	0.30271	266.76002	292.91402
17	C	5.0707	87.51367	-1468.74195	35.77250	-1432.96944	-1345.45578
18	H	-3.6547	26.20700	266.23876	0.44131	266.68007	292.88707
19	C	5.0557	84.47033	-1464.39713	35.84892	-1428.54821	-1344.07788
20	C	5.0770	86.04233	-1470.57643	35.65713	-1434.91929	-1348.87696
21	H	-3.6537	26.13133	266.16591	-0.05286	266.11305	292.24439
C Average		5.0659	87.10797	-1467.37092	35.79184	-1431.57908	-1344.47111
H Average		-3.6556	26.06523	266.30918	0.27113	266.58032	292.64555

```

=====
4VCp2-STO-PBE0-DZ-DZ
Temperature: 298
Spin: 1.5

```

```

atensor 1 V
-22.242 0.002 0.001
0.002 -22.232 -0.001
0.001 -0.001 -72.643
-8.627 0.001 0.000
0.001 -8.629 0.000
0.000 0.000 -3.182

```

atensor 2 H
1.051 -1.336 -1.360
-1.336 4.332 3.827
-1.360 3.827 4.335
0.021 0.008 0.011
0.008 0.000 -0.032
0.003 -0.009 -0.001

atensor 3 C
-1.602 -0.270 -0.617
-0.270 -0.951 1.754
-0.617 1.754 0.238
0.047 0.006 0.009
0.006 0.032 -0.025
0.006 -0.017 0.000

atensor 4 H
4.826 0.116 -4.057
0.116 0.612 -0.111
-4.057 -0.111 4.365
-0.003 -0.001 0.034
-0.001 0.024 0.001
0.009 0.000 -0.001

atensor 5 C
-0.848 0.024 -1.865
0.024 -1.697 -0.052
-1.865 -0.052 0.229
0.030 -0.001 0.027
-0.001 0.049 0.001
0.018 0.000 0.000

atensor 6 H
0.921 1.148 -1.148
1.148 4.473 -3.895
-1.148 -3.895 4.341
0.022 -0.007 0.010
-0.007 -0.001 0.033
0.003 0.009 -0.001

atensor 7 C
-1.633 0.233 -0.523
0.233 -0.926 -1.785
-0.523 -1.785 0.232
0.048 -0.005 0.008
-0.005 0.031 0.026
0.005 0.017 0.000

atensor 8 H
3.435 -1.978 3.351
-1.978 1.909 -2.295
3.350 -2.295 4.317
0.006 0.012 -0.028
0.012 0.015 0.019
-0.008 0.005 -0.001

atensor 9 C
-1.118 -0.398 1.551
-0.398 -1.427 -1.050
1.551 -1.050 0.273
0.036 0.009 -0.022
0.009 0.043 0.015
-0.015 0.010 0.000

atensor 10 H
3.212 2.049 3.219

2.049 2.126 2.475
3.219 2.475 4.315
0.007 -0.013 -0.027
-0.013 0.014 -0.021
-0.007 -0.006 -0.001

atensor 11 C
-1.163 0.414 1.493
0.414 -1.385 1.137
1.493 1.137 0.277
0.037 -0.009 -0.021
-0.009 0.042 -0.016
-0.014 -0.011 0.000

atensor 12 H
0.921 1.147 1.148
1.147 4.473 3.895
1.148 3.895 4.342
0.022 -0.007 -0.010
-0.007 -0.001 -0.033
-0.003 -0.009 -0.001

atensor 13 C
-1.632 0.233 0.522
0.233 -0.926 1.785
0.522 1.785 0.233
0.048 -0.005 -0.008
-0.005 0.031 -0.026
-0.005 -0.017 0.000

atensor 14 H
3.436 -1.977 -3.351
-1.977 1.909 2.295
-3.351 2.295 4.319
0.006 0.012 0.028
0.012 0.015 -0.019
0.008 -0.005 -0.001

atensor 15 C
-1.118 -0.398 -1.552
-0.398 -1.427 1.049
-1.552 1.049 0.272
0.036 0.009 0.022
0.009 0.043 -0.015
0.015 -0.010 0.000

atensor 16 H
3.211 2.050 -3.219
2.050 2.126 -2.475
-3.219 -2.475 4.314
0.007 -0.013 0.027
-0.013 0.014 0.021
0.007 0.006 -0.001

atensor 17 C
-1.163 0.414 -1.493
0.414 -1.385 -1.137
-1.493 -1.137 0.277
0.037 -0.009 0.021
-0.009 0.042 0.016
0.014 0.011 0.000

atensor 18 H
1.052 -1.336 1.360
-1.336 4.333 -3.827
1.360 -3.827 4.335
0.021 0.008 -0.011

0.008 0.000 0.032
-0.003 0.009 -0.001

atensor 19 C
-1.602 -0.270 0.617
-0.270 -0.951 -1.755
0.617 -1.754 0.237
0.047 0.006 -0.009
0.006 0.032 0.025
-0.006 0.017 0.000

atensor 20 C
-0.847 0.024 1.865
0.024 -1.697 0.052
1.865 0.052 0.228
0.030 -0.001 -0.027
-0.001 0.049 -0.001
-0.018 0.000 0.000

atensor 21 H
4.825 0.115 4.058
0.115 0.612 0.111
4.057 0.111 4.365
-0.003 -0.001 -0.034
-0.001 0.024 -0.001
-0.009 0.000 -0.001

orbtensor 1 V
-3505.948 0.483 0.851
0.483 -3505.905 -0.440
0.851 -0.440 -170.747
1708.423 -0.001 -0.002
-0.001 1708.420 -0.001
-0.002 -0.001 1723.127

orbtensor 2 H
2.884 4.405 0.852
4.405 -7.863 -2.369
0.852 -2.369 2.850
24.264 -5.300 -0.948
-5.300 37.305 2.666
-0.948 2.666 24.069

orbtensor 3 C
-156.646 14.900 9.747
14.900 -191.656 -23.815
9.747 -23.815 -51.992
254.201 7.623 -0.754
7.623 235.584 2.161
-0.754 2.161 242.666

orbtensor 4 H
-9.450 -0.317 2.522
-0.317 4.519 -0.012
2.522 -0.012 2.853
39.148 0.460 -2.829
0.460 22.385 -0.078
-2.829 -0.078 24.060

orbtensor 5 C
-196.815 -1.120 26.861
-1.120 -154.130 0.125
26.861 0.125 -52.112
232.778 -0.667 -2.268
-0.667 256.912 -0.059
-2.268 -0.059 242.673

```

orbtensor 6 H
3.307   -3.751   0.729
-3.751  -8.250   2.361
0.729   2.361   2.855
23.717   4.554  -0.800
4.554   37.841 -2.714
-0.800  -2.714  24.063

orbtensor 7 C
-157.636 -11.093   6.824
-11.093 -191.895 25.813
6.824   25.813 -52.712
254.968 -6.563  -0.632
-6.563  234.786 -2.198
-0.632  -2.198 242.652

orbtensor 8 H
-5.094   6.415  -2.112
6.415  -0.072   1.480
-2.112  1.480   2.852
33.814  -7.838  2.328
-7.838  27.749 -1.596
2.328  -1.596  24.062

orbtensor 9 C
-180.739  22.252 -22.193
22.252 -165.813 14.660
-22.193  14.660 -51.756
240.586  11.216  1.880
11.216  249.262 -1.282
1.880  -1.282 242.659

orbtensor 10 H
-4.246  -6.618  -2.001
-6.618  -0.778  -1.489
-2.001  -1.489  2.843
32.927   8.123  2.236
8.123  28.615  1.721
2.236  1.721  24.050

orbtensor 11 C
-179.768 -22.309 -19.905
-22.309 -164.829 -14.710
-19.905 -14.710 -52.780
241.828 -11.630  1.802
-11.630  248.004  1.381
1.802   1.381 242.637

orbtensor 12 H
3.310  -3.672  -0.710
-3.672  -8.259  -2.380
-0.710  -2.380  2.847
23.718   4.553  0.801
4.553   37.840  2.716
0.801   2.716  24.064

orbtensor 13 C
-153.185 -12.689  -6.490
-12.689 -191.907 -23.979
-6.490 -23.979 -52.622
254.967  -6.563  0.632
-6.563  234.784  2.198
0.632   2.198 242.652

orbtensor 14 H
-5.040   6.571   2.078
6.571   0.020  -1.473

```

2.078	-1.473	2.850
33.815	-7.837	-2.328
-7.837	27.749	1.596
-2.328	1.596	24.063

orbtensor 15 C

-184.591	20.809	22.143
20.809	-167.113	-14.833
22.143	-14.833	-51.682
240.586	11.217	-1.880
11.217	249.260	1.283
-1.880	1.283	242.657

orbtensor 16 H

-4.318	-6.722	1.998
-6.722	-0.603	1.447
1.998	1.447	2.849
32.927	8.123	-2.235
8.123	28.617	-1.720
-2.235	-1.720	24.049

orbtensor 17 C

-181.679	-19.419	21.348
-19.419	-170.585	16.012
21.348	16.012	-52.784
241.826	-11.631	-1.803
-11.631	248.007	-1.380
-1.803	-1.380	242.632

orbtensor 18 H

2.799	4.345	-0.851
4.345	-7.861	2.385
-0.851	2.385	2.855
24.264	-5.300	0.947
-5.300	37.306	-2.665
0.947	-2.665	24.069

orbtensor 19 C

-156.675	13.412	-10.369
13.412	-191.209	24.870
-10.369	24.870	-52.065
254.200	7.622	0.755
7.622	235.585	-2.162
0.755	-2.162	242.667

orbtensor 20 C

-195.572	0.557	-25.702
0.557	-147.358	-0.070
-25.702	-0.070	-52.140
232.775	-0.669	2.268
-0.669	256.909	0.060
2.268	0.060	242.672

orbtensor 21 H

-9.347	-0.389	-2.562
-0.389	4.259	-0.017
-2.562	-0.017	2.852
39.147	0.459	2.829
0.459	22.384	0.078
2.829	0.078	24.060

gtensor (ppt)

-0.152	0.000	0.000
0.000	-0.152	0.000
0.000	0.000	-0.132
-11.011	-0.007	-0.008
-0.007	-11.022	-0.006

-0.008 -0.006 -0.782

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-45.8517	-680.87667	22979.96938	25.74386	23005.71324	22324.83657
2	H	3.2460	27.83633	-428.44520	-0.24559	-428.69078	-400.85445
3	C	-0.7453	110.71900	391.15981	-0.88345	390.27637	500.99537
4	H	3.2743	27.83833	-432.18496	-0.24841	-432.43337	-404.59504
5	C	-0.7457	109.76867	391.33475	-0.87962	390.45513	500.22380
6	H	3.2517	27.84433	-429.19315	-0.24683	-429.43998	-401.59564
7	C	-0.7493	110.05433	393.25906	-0.88457	392.37449	502.42883
8	H	3.2270	27.77033	-425.93735	-0.24655	-426.18390	-398.41357
9	C	-0.7310	111.39967	383.63751	-0.90255	382.73496	494.13463
10	H	3.2243	27.80367	-425.58537	-0.24420	-425.82958	-398.02591
11	C	-0.7307	111.69733	383.46257	-0.90264	382.55993	494.25727
12	H	3.2520	27.84000	-429.23715	-0.24412	-429.48127	-401.64127
13	C	-0.7487	111.56300	392.90919	-0.87971	392.02948	503.59248
14	H	3.2280	27.81900	-426.06934	-0.24792	-426.31726	-398.49826
15	C	-0.7313	109.70567	383.81245	-0.90407	382.90838	492.61404
16	H	3.2237	27.84033	-425.49738	-0.24769	-425.74507	-397.90474
17	C	-0.7307	109.13900	383.46257	-0.90915	382.55343	491.69243
18	H	3.2467	27.81067	-428.53319	-0.24650	-428.77969	-400.96902
19	C	-0.7457	110.83433	391.33475	-0.88479	390.44996	501.28430
20	C	-0.7457	112.42867	391.33475	-0.87344	390.46131	502.88998
21	H	3.2740	27.78500	-432.14096	-0.24558	-432.38654	-404.60154
	C Average	-0.7404	110.73097	388.57074	-0.89040	387.68034	498.41131
	H Average	3.2448	27.81880	-428.28241	-0.24634	-428.52874	-400.70994

4VCp2-STO-PBE0-DZ-TZ2P

Temperature: 298

Spin: 1.5

atensor 1 V

-7.838 0.002 -0.002
0.002 -7.816 0.002
-0.002 0.002 -59.597
-8.519 0.000 0.000
0.000 -8.515 0.000
0.000 0.000 -3.309

atensor 2 H

0.709 -1.360 -1.305
-1.360 4.052 3.676
-1.305 3.676 3.957
0.018 0.006 0.010
0.006 0.002 -0.028
0.003 -0.009 -0.002

atensor 3 C

-1.937 -0.263 -0.600
-0.263 -1.291 1.696
-0.600 1.696 -0.106
0.049 0.007 0.009
0.007 0.032 -0.025
0.006 -0.017 0.000

atensor 4 H

4.545 0.118 -3.899
0.118 0.247 -0.107
-3.899 -0.107 3.971
0.000 -0.001 0.030
-0.001 0.020 0.001
0.010 0.000 -0.002

atensor 5 C
-1.208 0.023 -1.798
0.023 -2.043 -0.050
-1.798 -0.050 -0.130
0.030 -0.001 0.026
-0.001 0.051 0.001
0.018 0.001 0.000

atensor 6 H
0.572 1.169 -1.102
1.169 4.193 -3.742
-1.102 -3.742 3.958
0.019 -0.006 0.008
-0.006 0.001 0.029
0.003 0.009 -0.002

atensor 7 C
-1.967 0.226 -0.506
0.226 -1.267 -1.727
-0.506 -1.727 -0.110
0.049 -0.006 0.007
-0.006 0.032 0.025
0.005 0.018 0.000

atensor 8 H
3.158 -2.011 3.220
-2.011 1.602 -2.206
3.220 -2.206 3.955
0.006 0.010 -0.025
0.010 0.014 0.017
-0.008 0.006 -0.002

atensor 9 C
-1.448 -0.389 1.484
-0.389 -1.748 -1.016
1.484 -1.016 -0.090
0.037 0.010 -0.021
0.010 0.044 0.015
-0.015 0.010 0.000

atensor 10 H
2.934 2.084 3.094
2.084 1.828 2.379
3.094 2.379 3.956
0.007 -0.010 -0.024
-0.010 0.013 -0.018
-0.008 -0.006 -0.002

atensor 11 C
-1.484 0.403 1.427
0.403 -1.698 1.096
1.427 1.096 -0.081
0.038 -0.010 -0.021
-0.010 0.043 -0.016
-0.015 -0.011 0.000

atensor 12 H
0.572 1.169 1.102
1.169 4.191 3.742
1.102 3.742 3.959

0.019 -0.006 -0.008
-0.006 0.001 -0.029
-0.003 -0.009 -0.002

atensor 13 C
-1.966 0.226 0.506
0.226 -1.266 1.727
0.506 1.727 -0.108
0.049 -0.006 -0.007
-0.006 0.032 -0.025
-0.005 -0.018 0.000

atensor 14 H
3.158 -2.010 -3.220
-2.010 1.602 2.205
-3.220 2.205 3.956
0.006 0.010 0.025
0.010 0.014 -0.017
0.008 -0.006 -0.002

atensor 15 C
-1.448 -0.389 -1.485
-0.389 -1.749 1.015
-1.484 1.015 -0.091
0.037 0.010 0.021
0.010 0.044 -0.015
0.015 -0.010 0.000

atensor 16 H
2.934 2.084 -3.094
2.084 1.828 -2.379
-3.094 -2.379 3.955
0.007 -0.010 0.024
-0.010 0.013 0.018
0.008 0.006 -0.002

atensor 17 C
-1.485 0.403 -1.427
0.403 -1.699 -1.096
-1.427 -1.096 -0.082
0.038 -0.010 0.021
-0.010 0.043 0.016
0.015 0.011 0.000

atensor 18 H
0.709 -1.360 1.305
-1.360 4.053 -3.676
1.305 -3.676 3.956
0.018 0.006 -0.010
0.006 0.002 0.028
-0.003 0.009 -0.002

atensor 19 C
-1.938 -0.263 0.600
-0.263 -1.291 -1.696
0.600 -1.696 -0.109
0.049 0.007 -0.009
0.007 0.032 0.025
-0.006 0.017 0.000

atensor 20 C
-1.208 0.023 1.798
0.023 -2.043 0.049
1.798 0.049 -0.131
0.030 -0.001 -0.026
-0.001 0.051 -0.001
-0.018 0.000 0.000

atensor 21 H
4.545 0.118 3.899
0.118 0.247 0.107
3.899 0.107 3.971
0.000 -0.001 -0.030
-0.001 0.020 -0.001
-0.010 0.000 -0.002

orbtensor 1 V
-3462.362 -0.040 -0.077
-0.040 -3467.540 -0.247
-0.077 -0.247 -223.533
1713.382 0.000 -0.001
0.000 1713.381 -0.001
-0.001 -0.001 1723.283

orbtensor 2 H
-0.424 4.376 1.242
4.376 -11.062 -3.420
1.242 -3.420 -0.035
26.365 -4.877 -1.262
-4.877 38.353 3.551
-1.262 3.551 25.089

orbtensor 3 C
-180.982 17.217 7.774
17.217 -221.776 -24.389
7.774 -24.389 -73.546
247.228 2.579 -2.137
2.579 240.902 6.015
-2.137 6.015 232.899

orbtensor 4 H
-12.574 -0.424 3.590
-0.424 1.013 0.185
3.590 0.185 -0.004
40.076 0.424 -3.766
0.424 24.643 -0.103
-3.766 -0.103 25.087

orbtensor 5 C
-226.986 -1.473 24.946
-1.473 -172.292 0.528
24.946 0.528 -73.466
239.994 -0.223 -6.380
-0.223 248.145 -0.175
-6.380 -0.175 232.905

orbtensor 6 H
0.095 -3.714 0.981
-3.714 -11.574 3.546
0.981 3.546 0.025
25.867 4.192 -1.065
4.192 38.851 -3.614
-1.065 -3.614 25.088

orbtensor 7 C
-179.459 -14.394 7.284
-14.394 -224.008 24.565
7.284 24.565 -73.990
247.490 -2.216 -1.804
-2.216 240.636 -6.124
-1.804 -6.124 232.895

orbtensor 8 H
-8.264 6.340 -2.990

6.340	-3.264	2.024
-2.990	2.024	0.002
35.145	-7.208	3.110
-7.208	29.569	-2.131
3.110	-2.131	25.086

orbtensor 9 C

-209.959	25.205	-20.179
25.205	-189.754	14.611
-20.179	14.611	-73.634
242.590	3.806	5.269
3.806	245.537	-3.609
5.269	-3.609	232.901

orbtensor 10 H

-7.474	-6.618	-2.841
-6.618	-4.059	-2.289
-2.841	-2.289	-0.030
34.339	7.470	2.989
7.470	30.375	2.299
2.989	2.299	25.088

orbtensor 11 C

-207.265	-25.896	-19.683
-25.896	-193.085	-15.508
-19.683	-15.508	-73.674
243.014	-3.944	5.064
-3.944	245.109	3.893
5.064	3.893	232.899

orbtensor 12 H

0.105	-3.714	-0.987
-3.714	-11.560	-3.569
-0.987	-3.569	0.002
25.867	4.192	1.066
4.192	38.851	3.615
1.066	3.615	25.089

orbtensor 13 C

-179.473	-14.382	-7.308
-14.382	-223.953	-24.614
-7.308	-24.614	-73.970
247.490	-2.215	1.805
-2.215	240.633	6.124
1.805	6.124	232.895

orbtensor 14 H

-8.269	6.339	2.984
6.339	-3.268	-2.020
2.984	-2.020	-0.004
35.144	-7.208	-3.110
-7.208	29.570	2.131
-3.110	2.131	25.086

orbtensor 15 C

-209.950	25.222	20.164
25.222	-189.746	-14.620
20.164	-14.620	-73.626
242.586	3.806	-5.269
3.806	245.539	3.609
-5.269	3.609	232.899

orbtensor 16 H

-7.475	-6.617	2.844
-6.617	-4.052	2.300
2.844	2.300	-0.026
34.342	7.470	-2.987

7.470 30.377 -2.297
 -2.987 -2.297 25.088

orbtensor 17 C
 -207.288 -25.885 19.682
 -25.885 -193.079 15.492
 19.682 15.492 -73.663
 243.022 -3.944 -5.063
 -3.944 245.115 -3.891
 -5.063 -3.891 232.901

orbtensor 18 H
 -0.423 4.378 -1.237
 4.378 -11.056 3.430
 -1.237 3.430 -0.040
 26.366 -4.877 1.261
 -4.877 38.355 -3.549
 1.261 -3.549 25.088

orbtensor 19 C
 -180.995 17.218 -7.776
 17.218 -221.762 24.370
 -7.776 24.370 -73.516
 247.232 2.579 2.137
 2.579 240.906 -6.013
 2.137 -6.013 232.897

orbtensor 20 C
 -227.022 -1.468 -24.947
 -1.468 -172.285 -0.542
 -24.947 -0.542 -73.429
 239.995 -0.224 6.380
 -0.224 248.146 0.176
 6.380 0.176 232.905

orbtensor 21 H
 -12.578 -0.424 -3.583
 -0.424 1.009 -0.184
 -3.583 -0.184 -0.025
 40.076 0.424 3.766
 0.424 24.643 0.103
 3.766 0.103 25.087

gtensor (ppt)
 -0.154 0.000 0.000
 0.000 -0.154 0.000
 0.000 0.000 -0.128
 -10.535 -0.011 0.000
 -0.011 -10.539 -0.001
 0.000 -0.001 -0.800

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
 Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-31.8647	-667.79633	15972.46668	25.38328	15997.84996	15330.05363
2	H	2.9120	26.09533	-384.42040	-0.22497	-384.64536	-358.55003
3	C	-1.0843	81.57500	569.16055	-0.83782	568.32273	649.89773
4	H	2.9270	26.08033	-386.40059	-0.22454	-386.62512	-360.54479
5	C	-1.1000	82.76667	577.38389	-0.83070	576.55319	659.31986
6	H	2.9137	26.11733	-384.64042	-0.22392	-384.86433	-358.74700
7	C	-1.0877	81.18800	570.91019	-0.83691	570.07328	651.26128

8	H	2.9110	26.09133	-384.28839	-0.22554	-384.51392	-358.42259
9	C	-1.0683	82.56033	560.76223	-0.83869	559.92355	642.48388
10	H	2.9120	26.07967	-384.42040	-0.22334	-384.64374	-358.56407
11	C	-1.0607	82.33267	556.73804	-0.83796	555.90009	638.23275
12	H	2.9133	26.11800	-384.59641	-0.22387	-384.82029	-358.70229
13	C	-1.0863	81.20733	570.21033	-0.83689	569.37345	650.58078
14	H	2.9113	26.08633	-384.33239	-0.22549	-384.55788	-358.47154
15	C	-1.0690	82.56733	561.11216	-0.83805	560.27411	642.84145
16	H	2.9117	26.08467	-384.37639	-0.22341	-384.59980	-358.51513
17	C	-1.0617	82.33600	557.26294	-0.83834	556.42460	638.76060
18	H	2.9120	26.09667	-384.42040	-0.22507	-384.64547	-358.54881
19	C	-1.0857	81.58733	569.86041	-0.83698	569.02343	650.61076
20	C	-1.1003	82.77000	577.55886	-0.83011	576.72874	659.49874
21	H	2.9270	26.07067	-386.40059	-0.22453	-386.62512	-360.55445
C Average		-1.0804	82.08907	567.09596	-0.83624	566.25972	648.34878
H Average		2.9151	26.09203	-384.82964	-0.22447	-385.05410	-358.96207

=====
4VCp2-STO-PBE0-DZ-QZ4P
Temperature: 298
Spin: 1.5

atensor 1 V
-1.550 0.002 0.000
0.002 -1.528 0.000
0.000 0.000 -53.788
-8.424 0.000 0.000
0.000 -8.421 -0.001
0.000 -0.001 -3.293

atensor 2 H
0.600 -1.360 -1.308
-1.360 3.942 3.682
-1.308 3.682 3.878
0.018 0.006 0.010
0.006 0.003 -0.028
0.003 -0.009 -0.002

atensor 3 C
-2.005 -0.255 -0.592
-0.255 -1.377 1.676
-0.592 1.676 -0.208
0.049 0.006 0.009
0.006 0.033 -0.024
0.006 -0.018 0.001

atensor 4 H
4.434 0.118 -3.905
0.118 0.137 -0.108
-3.905 -0.108 3.891
0.000 -0.001 0.029
-0.001 0.020 0.001
0.009 0.000 -0.002

atensor 5 C
-1.296 0.022 -1.777
0.022 -2.107 -0.049
-1.777 -0.049 -0.230
0.031 -0.001 0.026
-0.001 0.051 0.001
0.019 0.001 0.001

atensor 6 H
0.464 1.169 -1.104
1.169 4.083 -3.748

-1.104 -3.748 3.880
0.019 -0.005 0.008
-0.005 0.002 0.028
0.003 0.009 -0.002

atensor 7 C
-2.034 0.219 -0.500
0.219 -1.354 -1.707
-0.500 -1.707 -0.211
0.050 -0.006 0.007
-0.006 0.032 0.025
0.005 0.018 0.001

atensor 8 H
3.045 -2.010 3.225
-2.010 1.490 -2.210
3.225 -2.210 3.873
0.007 0.009 -0.024
0.009 0.014 0.017
-0.008 0.005 -0.002

atensor 9 C
-1.533 -0.378 1.466
-0.378 -1.825 -1.003
1.466 -1.003 -0.196
0.037 0.010 -0.021
0.010 0.045 0.015
-0.016 0.011 0.001

atensor 10 H
2.822 2.083 3.099
2.083 1.717 2.383
3.099 2.383 3.875
0.008 -0.010 -0.023
-0.010 0.013 -0.018
-0.008 -0.006 -0.002

atensor 11 C
-1.571 0.391 1.410
0.391 -1.779 1.083
1.410 1.083 -0.190
0.038 -0.010 -0.021
-0.010 0.044 -0.016
-0.015 -0.012 0.001

atensor 12 H
0.463 1.169 1.104
1.169 4.082 3.748
1.104 3.748 3.881
0.019 -0.005 -0.008
-0.005 0.002 -0.028
-0.003 -0.009 -0.002

atensor 13 C
-2.033 0.219 0.500
0.219 -1.353 1.706
0.500 1.706 -0.210
0.050 -0.006 -0.007
-0.006 0.032 -0.025
-0.005 -0.018 0.001

atensor 14 H
3.045 -2.009 -3.225
-2.009 1.490 2.209
-3.225 2.209 3.874
0.007 0.009 0.024
0.009 0.014 -0.017

0.008 -0.005 -0.002

atensor 15 C
-1.534 -0.378 -1.467
-0.378 -1.825 1.003
-1.467 1.003 -0.197
0.037 0.010 0.021
0.010 0.045 -0.015
0.016 -0.011 0.001

atensor 16 H
2.822 2.083 -3.099
2.083 1.717 -2.383
-3.099 -2.383 3.874
0.008 -0.010 0.023
-0.010 0.013 0.018
0.008 0.006 -0.002

atensor 17 C
-1.573 0.392 -1.410
0.392 -1.780 -1.083
-1.410 -1.083 -0.192
0.038 -0.010 0.021
-0.010 0.044 0.016
0.015 0.012 0.001

atensor 18 H
0.601 -1.360 1.308
-1.360 3.943 -3.682
1.308 -3.682 3.878
0.018 0.006 -0.010
0.006 0.003 0.028
-0.003 0.009 -0.002

atensor 19 C
-2.005 -0.255 0.592
-0.255 -1.377 -1.676
0.592 -1.676 -0.211
0.049 0.006 -0.009
0.006 0.033 0.024
-0.006 0.018 0.001

atensor 20 C
-1.296 0.022 1.777
0.022 -2.106 0.049
1.777 0.049 -0.231
0.031 -0.001 -0.026
-0.001 0.051 -0.001
-0.019 -0.001 0.001

atensor 21 H
4.434 0.118 3.905
0.118 0.137 0.107
3.905 0.107 3.891
0.000 -0.001 -0.029
-0.001 0.020 -0.001
-0.009 0.000 -0.002

orbtensor 1 V
-3358.456 -1.402 -0.093
-1.402 -3363.671 -0.296
-0.093 -0.296 -194.077
1695.391 0.000 0.000
0.000 1695.390 -0.001
0.000 -0.001 1726.770

orbtensor 2 H

1.626	5.797	0.900
5.797	-12.742	-2.780
0.900	-2.780	1.596
24.034	-6.415	-0.877
-6.415	39.799	2.467
-0.877	2.467	23.012

orbtensor 3 C

-187.163	19.846	7.274
19.846	-240.673	-21.480
7.274	-21.480	-72.166
251.106	-0.397	-1.386
-0.397	252.091	3.898
-1.386	3.898	231.277

orbtensor 4 H

-14.558	-0.507	2.695
-0.507	3.595	0.073
2.695	0.073	1.619
42.065	0.557	-2.616
0.557	21.770	-0.072
-2.616	-0.072	23.011

orbtensor 5 C

-244.400	-1.915	23.090
-1.915	-181.533	0.633
23.090	0.633	-72.219
252.236	0.035	-4.137
0.035	250.974	-0.112
-4.137	-0.112	231.282

orbtensor 6 H

2.272	-5.019	0.738
-5.019	-13.287	2.822
0.738	2.822	1.633
23.380	5.513	-0.740
5.513	40.455	-2.511
-0.740	-2.511	23.011

orbtensor 7 C

-185.948	-16.181	6.142
-16.181	-242.541	21.660
6.142	21.660	-72.220
251.065	0.342	-1.170
0.342	252.130	-3.967
-1.170	-3.967	231.273

orbtensor 8 H

-8.718	8.588	-2.237
8.588	-2.246	1.714
-2.237	1.714	1.603
35.581	-9.480	2.161
-9.480	28.248	-1.481
2.161	-1.481	23.009

orbtensor 9 C

-223.780	29.522	-18.289
29.522	-203.077	12.036
-18.289	12.036	-72.226
251.823	-0.592	3.413
-0.592	251.368	-2.339
3.413	-2.339	231.275

orbtensor 10 H

-7.681	-8.921	-2.081
-8.921	-3.151	-1.783
-2.081	-1.783	1.586

34.521	9.824	2.077
9.824	29.308	1.598
2.077	1.598	23.009

orbtensor 11 C

-220.845	-29.837	-18.257
-29.837	-206.832	-12.962
-18.257	-12.962	-72.172
251.754	0.614	3.280
0.614	251.433	2.524
3.280	2.524	231.272

orbtensor 12 H

2.271	-5.017	-0.742
-5.017	-13.289	-2.819
-0.742	-2.819	1.624
23.381	5.512	0.740
5.512	40.455	2.512
0.740	2.512	23.013

orbtensor 13 C

-185.945	-16.185	-6.160
-16.185	-242.546	-21.659
-6.160	-21.659	-72.225
251.068	0.341	1.171
0.341	252.132	3.970
1.171	3.970	231.276

orbtensor 14 H

-8.713	8.591	2.242
8.591	-2.242	-1.723
2.242	-1.723	1.623
35.583	-9.479	-2.161
-9.479	28.248	1.481
-2.161	1.481	23.010

orbtensor 15 C

-223.785	29.524	18.281
29.524	-203.075	-12.041
18.281	-12.041	-72.225
251.831	-0.591	-3.412
-0.591	251.369	2.341
-3.412	2.341	231.279

orbtensor 16 H

-7.682	-8.921	2.092
-8.921	-3.147	1.788
2.092	1.788	1.605
34.522	9.824	-2.075
9.824	29.309	-1.596
-2.075	-1.596	23.009

orbtensor 17 C

-220.824	-29.849	18.246
-29.849	-206.844	12.958
18.246	12.958	-72.165
251.756	0.614	-3.279
0.614	251.433	-2.521
-3.279	-2.521	231.270

orbtensor 18 H

1.633	5.805	-0.899
5.805	-12.740	2.777
-0.899	2.777	1.587
24.035	-6.415	0.876
-6.415	39.800	-2.465
0.876	-2.465	23.011

```

orbtensor 19 C
-187.153   19.854   -7.274
19.854 -240.683   21.441
-7.274   21.441  -72.154
251.108   -0.397   1.387
-0.397  252.093   -3.895
1.387   -3.895  231.276

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orbtensor 20 C
-244.404  -1.920  -23.090
-1.920 -181.532  -0.648
-23.090  -0.648  -72.229
252.237   0.035   4.137
0.035  250.977   0.115
4.137   0.115  231.283

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orbtensor 21 H
-14.559  -0.505  -2.699
-0.505   3.597  -0.081
-2.699  -0.081   1.583
42.065   0.557   2.616
0.557  21.771   0.072
2.616   0.072  23.011

```

```

gtensor (ppt)
-0.162   0.000   0.000
0.000  -0.162   0.000
0.000   0.000  -0.129
-10.809   0.001   0.000
0.001 -10.747  -0.001
0.000  -0.001  -1.062

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-25.6680	-599.55100	12864.69262	25.65030	12890.34291	12290.79191
2	H	2.8130	25.77500	-371.30394	-0.23065	-371.53459	-345.75959
3	C	-1.1690	78.15733	613.52358	-0.82389	612.69969	690.85703
4	H	2.8267	25.83400	-373.10788	-0.22554	-373.33342	-347.49942
5	C	-1.1833	78.78000	621.04611	-0.81387	620.23225	699.01225
6	H	2.8153	25.82133	-371.61193	-0.23120	-371.84313	-346.02180
7	C	-1.1720	77.91967	615.09807	-0.82469	614.27337	692.19304
8	H	2.8090	25.82567	-370.77596	-0.22733	-371.00329	-345.17762
9	C	-1.1570	78.46100	607.22565	-0.82190	606.40375	684.86475
10	H	2.8110	25.86400	-371.03995	-0.22762	-371.26757	-345.40357
11	C	-1.1523	78.20333	604.77646	-0.82303	603.95342	682.15676
12	H	2.8150	25.81833	-371.56793	-0.23116	-371.79909	-345.98076
13	C	-1.1710	77.92000	614.57324	-0.82410	613.74914	691.66914
14	H	2.8093	25.83633	-370.81996	-0.22728	-371.04724	-345.21090
15	C	-1.1577	78.46467	607.57554	-0.82127	606.75427	685.21893
16	H	2.8107	25.87200	-370.99595	-0.22768	-371.22363	-345.35163
17	C	-1.1540	78.20867	605.65117	-0.82312	604.82804	683.03671
18	H	2.8137	25.77533	-371.39194	-0.23083	-371.62277	-345.84743
19	C	-1.1700	78.16233	614.04841	-0.82276	613.22565	691.38798
20	C	-1.1833	78.77733	621.04611	-0.81300	620.23312	699.01045
21	H	2.8267	25.82267	-373.10788	-0.22553	-373.33341	-347.51074
C Average		-1.1670	78.30543	612.45643	-0.82116	611.63527	689.94070
H Average		2.8150	25.82447	-371.57233	-0.22848	-371.80081	-345.97635

=====
4VCp2-STO-PBE0-TZ2P-DZ
Temperature: 298
Spin: 1.5

atensor 1 V
-18.824 0.003 0.000
0.003 -18.822 -0.001
0.000 -0.001 -71.155
-8.642 0.001 0.000
0.001 -8.646 0.000
0.000 0.000 -3.269

atensor 2 H
0.994 -1.342 -1.356
-1.342 4.291 3.816
-1.356 3.816 4.281
0.021 0.008 0.011
0.008 0.000 -0.032
0.003 -0.009 -0.001

atensor 3 C
-1.673 -0.269 -0.617
-0.269 -1.023 1.747
-0.617 1.747 0.245
0.046 0.006 0.009
0.006 0.031 -0.025
0.006 -0.017 0.000

atensor 4 H
4.783 0.116 -4.048
0.116 0.546 -0.111
-4.048 -0.111 4.305
-0.003 -0.001 0.034
-0.001 0.024 0.001
0.009 0.000 -0.001

atensor 5 C
-0.918 0.024 -1.858
0.024 -1.766 -0.052
-1.858 -0.052 0.242
0.029 -0.001 0.027
-0.001 0.048 0.001
0.018 0.000 0.000

atensor 6 H
0.862 1.153 -1.145
1.153 4.433 -3.885
-1.145 -3.885 4.286
0.022 -0.007 0.010
-0.007 -0.001 0.033
0.003 0.009 -0.001

atensor 7 C
-1.702 0.232 -0.523
0.232 -0.998 -1.778
-0.523 -1.777 0.240
0.047 -0.005 0.008
-0.005 0.030 0.026
0.005 0.017 0.000

atensor 8 H
3.393 -1.986 3.340
-1.986 1.859 -2.288
3.340 -2.288 4.266
0.006 0.012 -0.028

0.012 0.015 0.019
-0.008 0.005 -0.001

atensor 9 C
-1.198 -0.397 1.545
-0.397 -1.507 -1.047
1.545 -1.047 0.267
0.035 0.009 -0.022
0.009 0.042 0.015
-0.014 0.010 0.000

atensor 10 H
3.169 2.058 3.209
2.058 2.078 2.467
3.209 2.467 4.266
0.007 -0.013 -0.027
-0.013 0.014 -0.021
-0.007 -0.006 -0.001

atensor 11 C
-1.245 0.413 1.487
0.413 -1.466 1.133
1.487 1.133 0.268
0.036 -0.009 -0.021
-0.009 0.041 -0.016
-0.014 -0.011 0.000

atensor 12 H
0.862 1.153 1.145
1.153 4.432 3.885
1.145 3.885 4.286
0.022 -0.007 -0.010
-0.007 -0.001 -0.033
-0.003 -0.009 -0.001

atensor 13 C
-1.702 0.232 0.522
0.232 -0.997 1.778
0.522 1.778 0.242
0.047 -0.005 -0.008
-0.005 0.030 -0.026
-0.005 -0.017 0.000

atensor 14 H
3.393 -1.986 -3.340
-1.986 1.859 2.287
-3.340 2.287 4.267
0.006 0.012 0.028
0.012 0.015 -0.019
0.008 -0.005 -0.001

atensor 15 C
-1.197 -0.397 -1.545
-0.397 -1.507 1.047
-1.545 1.047 0.266
0.035 0.009 0.022
0.009 0.042 -0.015
0.014 -0.010 0.000

atensor 16 H
3.168 2.059 -3.209
2.059 2.078 -2.467
-3.208 -2.467 4.264
0.007 -0.013 0.027
-0.013 0.014 0.021
0.007 0.006 -0.001

atensor 17 C
-1.245 0.413 -1.487
0.413 -1.466 -1.133
-1.487 -1.133 0.268
0.036 -0.009 0.021
-0.009 0.041 0.016
0.014 0.011 0.000

atensor 18 H
0.994 -1.342 1.356
-1.342 4.292 -3.816
1.356 -3.816 4.280
0.021 0.008 -0.011
0.008 0.000 0.032
-0.003 0.009 -0.001

atensor 19 C
-1.673 -0.269 0.617
-0.269 -1.023 -1.747
0.617 -1.747 0.243
0.046 0.006 -0.009
0.006 0.031 0.025
-0.006 0.017 0.000

atensor 20 C
-0.918 0.024 1.858
0.024 -1.766 0.052
1.858 0.052 0.242
0.029 -0.001 -0.027
-0.001 0.048 -0.001
-0.018 0.000 0.000

atensor 21 H
4.783 0.116 4.048
0.116 0.545 0.111
4.048 0.111 4.305
-0.003 -0.001 -0.034
-0.001 0.024 -0.001
-0.009 0.000 -0.001

orbtensor 1 V
-3494.048 -0.944 -0.651
-0.944 -3499.219 0.337
-0.651 0.337 -196.043
1706.645 -0.001 -0.002
-0.001 1706.645 -0.001
-0.002 -0.001 1723.533

orbtensor 2 H
2.993 4.526 0.972
4.526 -8.093 -2.605
0.972 -2.605 2.958
24.210 -5.238 -0.883
-5.238 37.092 2.480
-0.883 2.480 24.046

orbtensor 3 C
-159.759 14.881 7.197
14.881 -194.391 -21.440
7.197 -21.440 -51.829
253.033 7.527 -0.675
7.527 234.640 1.928
-0.675 1.928 242.852

orbtensor 4 H
-9.676 -0.374 2.789
-0.374 4.679 0.100

2.789	0.100	2.959
38.914	0.455	-2.633
0.455	22.347	-0.072
-2.633	-0.072	24.036

orbtensor 5 C

-200.215	-1.627	21.530
-1.627	-156.837	0.947
21.530	0.947	-52.229
231.866	-0.659	-2.024
-0.659	255.699	-0.052
-2.024	-0.052	242.855

orbtensor 6 H

3.402	-3.900	0.789
-3.900	-8.622	2.697
0.789	2.697	2.958
23.668	4.501	-0.745
4.501	37.622	-2.525
-0.745	-2.525	24.040

orbtensor 7 C

-159.096	-11.900	6.280
-11.900	-197.892	21.694
6.280	21.694	-51.718
253.787	-6.480	-0.564
-6.480	233.852	-1.962
-0.564	-1.962	242.837

orbtensor 8 H

-5.218	6.696	-2.312
6.696	-0.050	1.571
-2.312	1.571	2.949
33.644	-7.743	2.164
-7.743	27.656	-1.485
2.164	-1.485	24.040

orbtensor 9 C

-189.305	21.037	-19.114
21.037	-168.797	12.735
-19.114	12.735	-52.259
239.589	11.082	1.673
11.082	248.165	-1.144
1.673	-1.144	242.844

orbtensor 10 H

-4.434	-6.931	-2.174
-6.931	-0.762	-1.745
-2.174	-1.745	2.950
32.768	8.024	2.079
8.024	28.512	1.600
2.079	1.600	24.028

orbtensor 11 C

-185.845	-21.932	-18.668
-21.932	-170.315	-13.950
-18.668	-13.950	-51.946
240.818	-11.492	1.602
-11.492	246.924	1.230
1.602	1.230	242.825

orbtensor 12 H

3.535	-3.906	-0.746
-3.906	-8.532	-2.691
-0.746	-2.691	2.958
23.668	4.501	0.746
4.501	37.621	2.527

0.746	2.527	24.041
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orbtensor 13 C

-160.791	-11.676	-7.103
-11.676	-196.964	-21.972
-7.103	-21.972	-51.642
253.786	-6.480	0.564
-6.480	233.850	1.962
0.564	1.962	242.838

orbtensor 14 H

-5.207	6.674	2.302
6.674	0.050	-1.545
2.302	-1.545	2.951
33.645	-7.742	-2.164
-7.742	27.656	1.485
-2.164	1.485	24.041

orbtensor 15 C

-185.546	21.650	17.951
21.650	-169.167	-12.571
17.951	-12.571	-52.172
239.589	11.084	-1.672
11.084	248.163	1.144
-1.672	1.144	242.843

orbtensor 16 H

-4.511	-6.935	2.202
-6.935	-0.682	1.719
2.202	1.719	2.952
32.768	8.024	-2.077
8.024	28.513	-1.599
-2.077	-1.599	24.028

orbtensor 17 C

-183.543	-22.023	17.146
-22.023	-174.328	13.840
17.146	13.840	-51.929
240.816	-11.494	-1.603
-11.494	246.926	-1.229
-1.603	-1.229	242.819

orbtensor 18 H

2.996	4.558	-0.954
4.558	-8.138	2.641
-0.954	2.641	2.955
24.209	-5.238	0.882
-5.238	37.092	-2.479
0.882	-2.479	24.046

orbtensor 19 C

-163.673	14.053	-7.827
14.053	-196.819	21.431
-7.827	21.431	-51.927
253.032	7.526	0.676
7.526	234.641	-1.930
0.676	-1.930	242.853

orbtensor 20 C

-200.655	-1.461	-23.279
-1.461	-151.061	-0.799
-23.279	-0.799	-52.199
231.864	-0.660	2.024
-0.660	255.696	0.053
2.024	0.053	242.854

orbtensor 21 H

```

-9.747   -0.379   -2.791
-0.379   4.454   -0.115
-2.791   -0.115   2.956
38.913   0.454   2.634
0.454   22.347   0.072
2.634   0.072   24.035

```

gtensor (ppt)

```

-0.151   0.000   0.000
0.000   -0.151   0.000
0.000   0.000   -0.130
-11.067   0.002   0.011
0.002   -11.073   -0.002
0.011   -0.002   -0.781

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-43.1193	-684.16233	21610.20833	27.03284	21637.24117	20953.07884
2	H	3.1953	27.73533	-421.75042	-0.24535	-421.99578	-394.26045
3	C	-0.7913	108.18200	415.29408	-0.93507	414.35901	522.54101
4	H	3.2180	27.75300	-424.74219	-0.24533	-424.98751	-397.23451
5	C	-0.7883	107.04633	413.71967	-0.92839	412.79129	519.83762
6	H	3.2003	27.68933	-422.41037	-0.24633	-422.65671	-394.96737
7	C	-0.7943	107.25667	416.86849	-0.93482	415.93367	523.19034
8	H	3.1793	27.67367	-419.63859	-0.24865	-419.88724	-392.21357
9	C	-0.7870	106.74567	413.01994	-0.95634	412.06360	518.80926
10	H	3.1777	27.68733	-419.41861	-0.24887	-419.66748	-391.98015
11	C	-0.7887	107.48700	413.89461	-0.95814	412.93647	520.42347
12	H	3.2000	27.76367	-422.36638	-0.24683	-422.61321	-394.84954
13	C	-0.7933	107.02567	416.34369	-0.93648	415.40720	522.43287
14	H	3.1797	27.71200	-419.68259	-0.24517	-419.92776	-392.21576
15	C	-0.7870	107.90333	413.01994	-0.94882	412.07112	519.97445
16	H	3.1767	27.68933	-419.28662	-0.24598	-419.53260	-391.84326
17	C	-0.7887	106.92033	413.89461	-0.95325	412.94135	519.86169
18	H	3.1953	27.72000	-421.75042	-0.24711	-421.99753	-394.27753
19	C	-0.7920	106.03567	415.64395	-0.93743	414.70652	520.74219
20	C	-0.7883	108.83300	413.71967	-0.93544	412.78424	521.61724
21	H	3.2177	27.65267	-424.69819	-0.24929	-424.94748	-397.29481
C Average		-0.7899	107.34357	414.54187	-0.94242	413.59945	520.94301
H Average		3.1940	27.70763	-421.57444	-0.24689	-421.82133	-394.11370

4VCp2-STO-PBE0-TZ2P-TZ2P

Temperature: 298

Spin: 1.5

atensor 1 V

```

-5.017 0.001 -0.002
0.001 -4.998 0.001
-0.002 0.001 -58.265
-8.517 0.000 0.000
0.000 -8.514 0.000
0.000 0.000 -3.393

```

atensor 2 H

```

0.657 -1.365 -1.305
-1.365 4.011 3.672
-1.305 3.672 3.909

```


0.018 0.006 0.010
0.006 0.002 -0.028
0.003 -0.009 -0.002

atensor 3 C
-1.949 -0.262 -0.601
-0.262 -1.304 1.692
-0.601 1.692 -0.052
0.048 0.007 0.009
0.007 0.032 -0.024
0.006 -0.017 0.000

atensor 4 H
4.502 0.119 -3.896
0.119 0.187 -0.107
-3.895 -0.107 3.918
0.000 -0.001 0.030
-0.001 0.020 0.001
0.010 0.000 -0.002

atensor 5 C
-1.213 0.023 -1.794
0.023 -2.045 -0.050
-1.794 -0.050 -0.065
0.030 -0.001 0.026
-0.001 0.050 0.001
0.018 0.001 0.000

atensor 6 H
0.519 1.173 -1.102
1.173 4.151 -3.738
-1.102 -3.738 3.910
0.019 -0.005 0.008
-0.005 0.002 0.029
0.003 0.009 -0.002

atensor 7 C
-1.975 0.226 -0.508
0.226 -1.277 -1.722
-0.508 -1.722 -0.053
0.049 -0.006 0.007
-0.006 0.031 0.025
0.005 0.018 0.000

atensor 8 H
3.116 -2.017 3.215
-2.017 1.556 -2.203
3.215 -2.203 3.911
0.006 0.009 -0.025
0.009 0.014 0.017
-0.008 0.006 -0.002

atensor 9 C
-1.478 -0.388 1.480
-0.388 -1.778 -1.015
1.480 -1.015 -0.057
0.036 0.010 -0.021
0.010 0.044 0.015
-0.015 0.010 0.000

atensor 10 H
2.893 2.090 3.089
2.090 1.784 2.376
3.089 2.376 3.913
0.007 -0.010 -0.024
-0.010 0.013 -0.018
-0.008 -0.006 -0.002

atensor 11 C
-1.518 0.402 1.423
0.402 -1.731 1.095
1.423 1.095 -0.052
0.037 -0.010 -0.021
-0.010 0.043 -0.016
-0.015 -0.011 0.000

atensor 12 H
0.518 1.173 1.102
1.173 4.150 3.738
1.102 3.738 3.910
0.019 -0.005 -0.008
-0.005 0.002 -0.029
-0.003 -0.009 -0.002

atensor 13 C
-1.974 0.225 0.508
0.225 -1.276 1.723
0.508 1.723 -0.051
0.049 -0.006 -0.007
-0.006 0.031 -0.025
-0.005 -0.018 0.000

atensor 14 H
3.116 -2.016 -3.215
-2.016 1.556 2.203
-3.215 2.203 3.911
0.006 0.009 0.025
0.009 0.014 -0.017
0.008 -0.006 -0.002

atensor 15 C
-1.478 -0.388 -1.480
-0.388 -1.778 1.015
-1.480 1.015 -0.057
0.036 0.010 0.021
0.010 0.044 -0.015
0.015 -0.010 0.000

atensor 16 H
2.892 2.090 -3.089
2.090 1.784 -2.376
-3.089 -2.376 3.912
0.007 -0.010 0.024
-0.010 0.013 0.018
0.008 0.006 -0.002

atensor 17 C
-1.518 0.403 -1.423
0.403 -1.732 -1.095
-1.423 -1.095 -0.053
0.037 -0.010 0.021
-0.010 0.043 0.016
0.015 0.011 0.000

atensor 18 H
0.657 -1.365 1.305
-1.365 4.012 -3.672
1.305 -3.672 3.909
0.018 0.006 -0.010
0.006 0.002 0.028
-0.003 0.009 -0.002

atensor 19 C
-1.949 -0.262 0.601

-0.262 -1.304 -1.692
0.601 -1.692 -0.055
0.048 0.007 -0.009
0.007 0.032 0.024
-0.006 0.017 0.000

atensor 20 C
-1.213 0.023 1.794
0.023 -2.046 0.049
1.794 0.049 -0.066
0.030 -0.001 -0.026
-0.001 0.050 -0.001
-0.018 -0.001 0.000

atensor 21 H
4.502 0.118 3.896
0.118 0.187 0.107
3.895 0.107 3.918
0.000 -0.001 -0.030
-0.001 0.020 -0.001
-0.010 0.000 -0.002

orbtensor 1 V
-3404.527 2.420 -0.083
2.420 -3397.547 -0.243
-0.083 -0.243 -213.077
1705.828 0.001 -0.001
0.001 1705.826 -0.001
-0.001 -0.001 1723.052

orbtensor 2 H
-1.232 4.402 0.945
4.402 -11.944 -2.880
0.945 -2.880 0.079
27.071 -5.003 -1.051
-5.003 39.365 2.956
-1.051 2.956 25.109

orbtensor 3 C
-184.896 16.340 7.512
16.340 -227.133 -22.151
7.512 -22.151 -74.952
253.720 2.441 -1.557
2.441 247.733 4.383
-1.557 4.383 233.225

orbtensor 4 H
-13.542 -0.319 3.035
-0.319 0.410 0.097
3.035 0.097 -0.008
41.133 0.435 -3.135
0.435 25.303 -0.086
-3.135 -0.086 25.107

orbtensor 5 C
-233.247 -2.112 23.560
-2.112 -180.201 0.966
23.560 0.966 -73.801
246.875 -0.211 -4.649
-0.211 254.588 -0.128
-4.649 -0.128 233.230

orbtensor 6 H
-0.857 -3.782 0.863
-3.782 -12.474 2.923
0.863 2.923 -0.006
26.560 4.300 -0.887

4.300 39.876 -3.008
-0.887 -3.008 25.108

orbtensor 7 C
-183.624 -15.399 6.841
-15.399 -229.091 22.565
6.841 22.565 -74.418
253.968 -2.098 -1.315
-2.098 247.481 -4.463
-1.315 -4.463 233.221

orbtensor 8 H
-9.037 6.481 -2.562
6.481 -3.979 1.731
-2.562 1.731 0.105
36.075 -7.392 2.588
-7.392 30.358 -1.774
2.588 -1.774 25.107

orbtensor 9 C
-215.039 24.178 -18.795
24.178 -196.850 12.692
-18.795 12.692 -75.427
249.330 3.603 3.838
3.603 252.119 -2.629
3.838 -2.629 233.226

orbtensor 10 H
-8.510 -6.690 -2.488
-6.690 -4.763 -1.858
-2.488 -1.858 0.138
35.249 7.660 2.487
7.660 31.185 1.913
2.487 1.913 25.108

orbtensor 11 C
-212.788 -26.364 -17.974
-26.364 -200.079 -14.245
-17.974 -14.245 -76.268
249.733 -3.734 3.688
-3.734 251.715 2.836
3.688 2.836 233.226

orbtensor 12 H
-0.857 -3.782 -0.863
-3.782 -12.473 -2.923
-0.863 -2.923 -0.007
26.560 4.300 0.887
4.300 39.875 3.010
0.887 3.010 25.109

orbtensor 13 C
-183.628 -15.394 -6.848
-15.394 -229.069 -22.581
-6.848 -22.581 -74.420
253.967 -2.096 1.316
-2.096 247.478 4.463
1.316 4.463 233.221

orbtensor 14 H
-9.038 6.481 2.562
6.481 -3.981 -1.731
2.562 -1.731 0.105
36.074 -7.392 -2.588
-7.392 30.358 1.774
-2.588 1.774 25.107

orbtensor 15 C
-215.028 24.180 18.792
24.180 -196.849 -12.708
18.792 -12.708 -75.413
249.325 3.604 -3.837
3.604 252.119 2.631
-3.837 2.631 233.224

orbtensor 16 H
-8.513 -6.690 2.487
-6.690 -4.764 1.857
2.487 1.857 0.138
35.251 7.661 -2.486
7.661 31.186 -1.912
-2.486 -1.912 25.109

orbtensor 17 C
-212.825 -26.364 17.971
-26.364 -200.083 14.228
17.971 14.228 -76.258
249.739 -3.734 -3.687
-3.734 251.719 -2.834
-3.687 -2.834 233.228

orbtensor 18 H
-1.234 4.402 -0.944
4.402 -11.946 2.878
-0.944 2.878 0.080
27.071 -5.003 1.050
-5.003 39.366 -2.954
1.050 -2.954 25.108

orbtensor 19 C
-184.904 16.343 -7.516
16.343 -227.133 22.131
-7.516 22.131 -74.945
253.722 2.441 1.558
2.441 247.735 -4.381
1.558 -4.381 233.223

orbtensor 20 C
-233.255 -2.107 -23.563
-2.107 -180.210 -0.982
-23.563 -0.982 -73.803
246.876 -0.212 4.649
-0.212 254.589 0.130
4.649 0.130 233.230

orbtensor 21 H
-13.542 -0.319 -3.035
-0.319 0.409 -0.097
-3.035 -0.097 -0.009
41.133 0.435 3.135
0.435 25.304 0.086
3.135 0.086 25.107

gtensor (ppt)
-0.149 0.000 0.000
0.000 -0.149 0.000
0.000 0.000 -0.126
-10.759 -0.002 0.000
-0.002 -10.764 -0.001
0.000 -0.001 -0.917

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
 Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-29.5680	-626.81500	14819.86870	26.52167	14846.39038	14219.57538
2	H	2.8650	26.14933	-378.18080	-0.22658	-378.40738	-352.25804
3	C	-1.0750	82.56567	564.20930	-0.88501	563.32429	645.88995
4	H	2.8750	26.13433	-379.50080	-0.22682	-379.72762	-353.59329
5	C	-1.0810	82.48133	567.35837	-0.87947	566.47890	648.96023
6	H	2.8663	26.06900	-378.35680	-0.22659	-378.58339	-352.51439
7	C	-1.0750	82.51233	564.20930	-0.88456	563.32474	645.83707
8	H	2.8670	26.20967	-378.44480	-0.22716	-378.67196	-352.46230
9	C	-1.0777	82.45300	565.60889	-0.88371	564.72518	647.17818
10	H	2.8693	26.13567	-378.75280	-0.22650	-378.97931	-352.84364
11	C	-1.0737	81.84633	563.50950	-0.88392	562.62559	644.47192
12	H	2.8657	26.06900	-378.26880	-0.22641	-378.49521	-352.42621
13	C	-1.0737	82.51633	563.50950	-0.88454	562.62496	645.14130
14	H	2.8670	26.20833	-378.44480	-0.22697	-378.67177	-352.46344
15	C	-1.0777	82.45933	565.60889	-0.88335	564.72553	647.18487
16	H	2.8687	26.13567	-378.66480	-0.22664	-378.89144	-352.75577
17	C	-1.0743	81.84000	563.85940	-0.88401	562.97539	644.81539
18	H	2.8653	26.14833	-378.22480	-0.22683	-378.45163	-352.30329
19	C	-1.0760	82.56600	564.73414	-0.88387	563.85028	646.41628
20	C	-1.0817	82.47567	567.70827	-0.87917	566.82910	649.30477
21	H	2.8750	26.13400	-379.50080	-0.22681	-379.72761	-353.59361
C Average		-1.0766	82.37160	565.03156	-0.88316	564.14840	646.52000
H Average		2.8684	26.13933	-378.63400	-0.22673	-378.86073	-352.72140

=====
 4VCp2-STO-PBE0-TZ2P-QZ4P
 Temperature: 298
 Spin: 1.5

atensor 1 V
 -0.823 0.001 0.000
 0.001 -0.803 -0.001
 0.000 -0.001 -54.120
 -8.448 0.000 0.000
 0.000 -8.445 -0.001
 0.000 -0.001 -3.411

atensor 2 H
 0.560 -1.361 -1.306
 -1.361 3.903 3.676
 -1.306 3.675 3.836
 0.018 0.006 0.010
 0.006 0.003 -0.028
 0.003 -0.009 -0.002

atensor 3 C
 -2.027 -0.255 -0.594
 -0.255 -1.401 1.673
 -0.594 1.673 -0.171
 0.048 0.006 0.009
 0.006 0.033 -0.024
 0.006 -0.018 0.001

atensor 4 H
 4.392 0.118 -3.899
 0.118 0.090 -0.108
 -3.899 -0.108 3.843
 0.001 -0.001 0.029
 -0.001 0.020 0.001

0.010 0.000 -0.002

atensor 5 C
-1.314 0.022 -1.774
0.022 -2.122 -0.049
-1.773 -0.049 -0.184
0.030 -0.001 0.026
-0.001 0.051 0.001
0.019 0.001 0.001

atensor 6 H
0.422 1.170 -1.103
1.170 4.044 -3.741
-1.103 -3.741 3.837
0.019 -0.005 0.008
-0.005 0.002 0.028
0.003 0.009 -0.002

atensor 7 C
-2.054 0.219 -0.502
0.219 -1.375 -1.703
-0.502 -1.703 -0.172
0.049 -0.005 0.007
-0.005 0.032 0.025
0.005 0.018 0.001

atensor 8 H
3.008 -2.010 3.218
-2.010 1.453 -2.205
3.218 -2.205 3.835
0.007 0.009 -0.024
0.009 0.014 0.017
-0.008 0.005 -0.002

atensor 9 C
-1.571 -0.377 1.463
-0.377 -1.862 -1.004
1.463 -1.004 -0.176
0.037 0.009 -0.021
0.009 0.044 0.015
-0.016 0.011 0.001

atensor 10 H
2.786 2.083 3.092
2.083 1.681 2.378
3.092 2.378 3.838
0.008 -0.010 -0.023
-0.009 0.013 -0.018
-0.008 -0.006 -0.002

atensor 11 C
-1.611 0.391 1.407
0.391 -1.819 1.083
1.407 1.083 -0.174
0.038 -0.010 -0.020
-0.010 0.043 -0.016
-0.015 -0.012 0.001

atensor 12 H
0.422 1.170 1.103
1.170 4.042 3.741
1.103 3.741 3.838
0.019 -0.005 -0.008
-0.005 0.002 -0.028
-0.003 -0.009 -0.002

atensor 13 C

-2.053 0.219 0.502
0.219 -1.374 1.703
0.502 1.703 -0.170
0.049 -0.005 -0.007
-0.005 0.032 -0.025
-0.005 -0.018 0.001

atensor 14 H
3.008 -2.010 -3.218
-2.010 1.453 2.205
-3.218 2.205 3.835
0.007 0.009 0.024
0.009 0.014 -0.017
0.008 -0.005 -0.002

atensor 15 C
-1.571 -0.377 -1.464
-0.377 -1.862 1.004
-1.464 1.004 -0.177
0.037 0.009 0.021
0.009 0.044 -0.015
0.016 -0.011 0.001

atensor 16 H
2.786 2.084 -3.092
2.084 1.681 -2.378
-3.092 -2.378 3.837
0.008 -0.010 0.023
-0.009 0.013 0.018
0.008 0.006 -0.002

atensor 17 C
-1.612 0.391 -1.407
0.391 -1.819 -1.083
-1.407 -1.083 -0.175
0.038 -0.010 0.020
-0.010 0.043 0.016
0.015 0.012 0.001

atensor 18 H
0.560 -1.361 1.306
-1.361 3.904 -3.676
1.306 -3.675 3.836
0.018 0.006 -0.010
0.006 0.003 0.028
-0.003 0.009 -0.002

atensor 19 C
-2.028 -0.255 0.594
-0.255 -1.401 -1.673
0.594 -1.673 -0.174
0.048 0.006 -0.009
0.006 0.033 0.024
-0.006 0.018 0.001

atensor 20 C
-1.314 0.022 1.773
0.022 -2.122 0.049
1.773 0.049 -0.185
0.030 -0.001 -0.026
-0.001 0.051 -0.001
-0.019 -0.001 0.001

atensor 21 H
4.391 0.118 3.899
0.118 0.089 0.107
3.899 0.107 3.843

0.001 -0.001 -0.029
-0.001 0.020 -0.001
-0.010 0.000 -0.002

orbtensor 1 V
-3421.937 9.585 -0.084
9.585 -3397.928 -0.288
-0.084 -0.288 -243.757
1697.404 0.001 0.000
0.001 1697.402 -0.001
0.000 -0.001 1727.291

orbtensor 2 H
1.766 5.995 1.015
5.995 -12.809 -2.472
1.015 -2.472 1.205
24.033 -6.466 -0.874
-6.466 39.922 2.459
-0.874 2.459 23.015

orbtensor 3 C
-193.306 20.115 7.837
20.115 -240.452 -26.474
7.837 -26.474 -65.155
251.642 -0.430 -1.405
-0.430 252.705 3.954
-1.405 3.954 231.196

orbtensor 4 H
-15.092 -0.464 2.776
-0.464 3.709 0.023
2.776 0.023 1.206
42.207 0.562 -2.608
0.562 21.750 -0.072
-2.608 -0.072 23.014

orbtensor 5 C
-248.694 -1.737 27.177
-1.737 -182.462 2.223
27.177 2.223 -65.191
252.864 0.039 -4.196
0.039 251.496 -0.114
-4.196 -0.114 231.199

orbtensor 6 H
2.466 -5.146 0.719
-5.146 -13.391 2.565
0.719 2.565 1.203
23.372 5.557 -0.738
5.557 40.583 -2.503
-0.738 -2.503 23.015

orbtensor 7 C
-192.240 -16.374 8.613
-16.374 -242.958 24.456
8.613 24.456 -65.312
251.594 0.371 -1.186
0.371 252.747 -4.024
-1.186 -4.024 231.192

orbtensor 8 H
-9.085 8.769 -2.300
8.769 -2.240 1.490
-2.300 1.490 1.208
35.670 -9.555 2.153
-9.555 28.281 -1.476
2.153 -1.476 23.014

orbtensor 9 C
-228.160 30.364 -23.560
30.364 -203.212 15.849
-23.560 15.849 -65.072
252.416 -0.639 3.462
-0.639 251.923 -2.373
3.462 -2.373 231.197

orbtensor 10 H
-8.069 -9.101 -2.212
-9.101 -3.068 -1.606
-2.212 -1.606 1.202
34.603 9.901 2.070
9.901 29.350 1.592
2.070 1.592 23.015

orbtensor 11 C
-225.397 -30.349 -20.082
-30.349 -208.246 -16.063
-20.082 -16.063 -65.339
252.344 0.662 3.327
0.662 251.995 2.560
3.327 2.560 231.197

orbtensor 12 H
2.465 -5.145 -0.721
-5.145 -13.392 -2.567
-0.721 -2.567 1.202
23.374 5.557 0.739
5.557 40.583 2.504
0.739 2.504 23.016

orbtensor 13 C
-192.238 -16.366 -8.611
-16.366 -242.953 -24.476
-8.611 -24.476 -65.316
251.597 0.370 1.187
0.370 252.748 4.027
1.187 4.027 231.195

orbtensor 14 H
-9.086 8.769 2.302
8.769 -2.239 -1.489
2.302 -1.489 1.207
35.672 -9.554 -2.154
-9.554 28.281 1.476
-2.154 1.476 23.014

orbtensor 15 C
-228.180 30.365 23.557
30.365 -203.212 -15.852
23.557 -15.852 -65.089
252.424 -0.638 -3.461
-0.638 251.924 2.375
-3.461 2.375 231.201

orbtensor 16 H
-8.068 -9.100 2.211
-9.100 -3.068 1.605
2.211 1.605 1.202
34.604 9.901 -2.068
9.901 29.350 -1.591
-2.068 -1.591 23.014

orbtensor 17 C
-225.372 -30.350 20.069

```

-30.350  -208.237  16.046
20.069   16.046  -65.339
252.345   0.662  -3.326
0.662   251.995  -2.557
-3.326   -2.557  231.194

```

```

orbtensor 18 H
1.766    5.995   -1.014
5.995  -12.810    2.470
-1.014    2.470    1.207
24.033   -6.466    0.874
-6.466   39.923   -2.457
0.874   -2.457   23.015

```

```

orbtensor 19 C
-193.297  20.125   -7.826
20.125 -240.448   26.442
-7.826   26.442  -65.151
251.643  -0.431    1.405
-0.431  252.707  -3.951
1.405   -3.951  231.195

```

```

orbtensor 20 C
-248.688  -1.738  -27.175
-1.738 -182.454  -2.231
-27.175  -2.231 -65.189
252.866   0.038   4.195
0.038  251.499   0.117
4.195   0.117  231.200

```

```

orbtensor 21 H
-15.092  -0.463  -2.777
-0.463   3.709  -0.022
-2.777  -0.022   1.205
42.207   0.562   2.608
0.562   21.751   0.072
2.608   0.072  23.014

```

```

gtensor (ppt)
-0.158   0.000   0.000
0.000  -0.158   0.000
0.000   0.000  -0.127
-10.240  -0.071   0.000
-0.071 -10.408  -0.001
0.000  -0.001  -0.839

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-25.3500	-647.17500	12707.73500	25.64962	12733.38462	12086.20962
2	H	2.7727	25.71067	-366.04990	-0.22070	-366.27060	-340.55993
3	C	-1.1723	78.87667	615.39033	-0.83488	614.55545	693.43212
4	H	2.7813	25.59800	-367.19408	-0.23001	-367.42409	-341.82609
5	C	-1.1793	79.73733	619.06482	-0.83710	618.22772	697.96505
6	H	2.7740	25.74933	-366.22593	-0.21255	-366.43847	-340.68914
7	C	-1.1730	78.34100	615.74028	-0.82904	614.91124	693.25224
8	H	2.7717	25.61600	-365.91788	-0.23202	-366.14989	-340.53389
9	C	-1.1757	79.69733	617.14009	-0.84202	616.29807	695.99540
10	H	2.7747	25.67767	-366.31394	-0.21822	-366.53216	-340.85450
11	C	-1.1740	78.85133	616.26521	-0.83202	615.43319	694.28453
12	H	2.7737	25.74933	-366.18192	-0.21250	-366.39442	-340.64509

13	C	-1.1717	78.34433	615.04038	-0.82901	614.21137	692.55570
14	H	2.7717	25.61633	-365.91788	-0.23182	-366.14970	-340.53337
15	C	-1.1760	79.68933	617.31506	-0.84112	616.47395	696.16328
16	H	2.7743	25.67800	-366.26993	-0.21829	-366.48822	-340.81022
17	C	-1.1747	78.86200	616.61516	-0.83211	615.78306	694.64506
18	H	2.7730	25.71133	-366.09390	-0.22095	-366.31486	-340.60352
19	C	-1.1737	78.88300	616.09023	-0.83406	615.25618	694.13918
20	C	-1.1797	79.74467	619.23980	-0.83653	618.40327	698.14794
21	H	2.7807	25.59800	-367.10606	-0.23014	-367.33620	-341.73820
	C Average	-1.1750	79.10270	616.79014	-0.83479	615.95535	695.05805
	H Average	2.7748	25.67047	-366.32714	-0.22272	-366.54986	-340.87939

=====
4VCp2-STO-PBE0-QZ4P-DZ
Temperature: 298
Spin: 1.5

atensor 1 V
-32.179 0.001 -0.001
0.001 -32.184 -0.006
-0.001 -0.006 -89.172
-10.219 0.001 0.000
0.001 -10.224 -0.001
0.000 -0.001 -4.287

atensor 2 H
0.910 -1.344 -1.354
-1.344 4.210 3.813
-1.354 3.813 4.196
0.022 0.009 0.012
0.009 0.000 -0.035
0.003 -0.009 -0.001

atensor 3 C
-1.772 -0.270 -0.613
-0.270 -1.118 1.737
-0.613 1.737 0.203
0.048 0.007 0.010
0.007 0.032 -0.027
0.006 -0.018 0.000

atensor 4 H
4.711 0.116 -4.044
0.116 0.471 -0.111
-4.044 -0.111 4.230
-0.003 -0.001 0.037
-0.001 0.026 0.001
0.010 0.000 -0.001

atensor 5 C
-1.015 0.024 -1.847
0.024 -1.869 -0.052
-1.847 -0.052 0.192
0.029 -0.001 0.029
-0.001 0.051 0.001
0.019 0.001 0.000

atensor 6 H
0.780 1.154 -1.144
1.154 4.353 -3.881
-1.144 -3.881 4.203
0.023 -0.008 0.010
-0.008 -0.001 0.035
0.003 0.010 -0.001

atensor 7 C
-1.801 0.234 -0.519
0.234 -1.092 -1.767
-0.519 -1.767 0.196
0.049 -0.006 0.008
-0.006 0.031 0.028
0.005 0.018 0.000

atensor 8 H
3.312 -1.988 3.337
-1.988 1.776 -2.285
3.336 -2.285 4.182
0.006 0.013 -0.030
0.013 0.016 0.021
-0.008 0.006 -0.001

atensor 9 C
-1.295 -0.399 1.535
-0.399 -1.606 -1.039
1.535 -1.039 0.225
0.036 0.010 -0.024
0.010 0.044 0.016
-0.015 0.010 0.000

atensor 10 H
3.088 2.060 3.206
2.060 1.996 2.464
3.206 2.464 4.182
0.007 -0.014 -0.029
-0.014 0.015 -0.022
-0.008 -0.006 -0.001

atensor 11 C
-1.342 0.415 1.478
0.415 -1.564 1.125
1.478 1.125 0.228
0.037 -0.010 -0.023
-0.010 0.042 -0.018
-0.015 -0.011 0.000

atensor 12 H
0.778 1.154 1.144
1.154 4.352 3.881
1.144 3.881 4.203
0.023 -0.008 -0.010
-0.008 -0.001 -0.035
-0.003 -0.010 -0.001

atensor 13 C
-1.800 0.233 0.519
0.233 -1.091 1.767
0.519 1.767 0.200
0.049 -0.006 -0.008
-0.006 0.031 -0.028
-0.005 -0.018 0.000

atensor 14 H
3.312 -1.988 -3.337
-1.988 1.776 2.285
-3.337 2.285 4.183
0.006 0.013 0.030
0.013 0.016 -0.021
0.008 -0.006 -0.001

atensor 15 C
-1.294 -0.399 -1.536
-0.399 -1.605 1.039

-1.536 1.039 0.227
0.036 0.010 0.024
0.010 0.044 -0.016
0.015 -0.010 0.000

atensor 16 H
3.088 2.061 -3.205
2.061 1.997 -2.464
-3.205 -2.464 4.181
0.007 -0.014 0.029
-0.014 0.015 0.022
0.008 0.006 -0.001

atensor 17 C
-1.342 0.415 -1.478
0.415 -1.564 -1.126
-1.478 -1.126 0.228
0.037 -0.010 0.023
-0.010 0.042 0.018
0.015 0.011 0.000

atensor 18 H
0.910 -1.344 1.354
-1.344 4.211 -3.813
1.354 -3.813 4.195
0.022 0.009 -0.012
0.009 0.000 0.035
-0.003 0.009 -0.001

atensor 19 C
-1.772 -0.270 0.612
-0.270 -1.118 -1.737
0.612 -1.737 0.201
0.048 0.007 -0.010
0.007 0.032 0.027
-0.006 0.018 0.000

atensor 20 C
-1.014 0.024 1.847
0.024 -1.868 0.051
1.847 0.051 0.195
0.029 -0.001 -0.029
-0.001 0.051 -0.001
-0.019 -0.001 0.000

atensor 21 H
4.710 0.116 4.044
0.116 0.469 0.111
4.044 0.111 4.229
-0.003 -0.001 -0.037
-0.001 0.026 -0.001
-0.010 0.000 -0.001

orbtensor 1 V
-3646.312 3.763 0.000
3.763 -3643.318 -0.221
0.000 -0.221 -183.555
1702.237 -0.001 -0.001
-0.001 1702.249 -0.001
-0.001 -0.001 1725.860

orbtensor 2 H
4.303 3.342 0.574
3.342 -3.971 -1.429
0.574 -1.429 2.601
22.974 -4.168 -0.523
-4.168 33.223 1.473

```

-0.523    1.473    24.301

orbtensor 3 C
-152.553   10.999    8.964
10.999  -180.787  -23.740
8.964   -23.740  -51.991
238.987    7.473   -1.711
7.473   220.747    4.847
-1.711    4.847   239.551

orbtensor 4 H
-5.098   -0.222    1.564
-0.222    5.532    0.057
1.564     0.057    2.619
34.661    0.362   -1.571
0.362    21.473   -0.043
-1.571   -0.043   24.285

orbtensor 5 C
-183.801  -1.291   25.544
-1.291  -148.783    0.388
25.544    0.388  -52.479
217.975   -0.658   -5.117
-0.658   241.644   -0.135
-5.117   -0.135  239.584

orbtensor 6 H
4.576   -2.903    0.386
-2.903   -4.284    1.436
0.386    1.436    2.601
22.540    3.582   -0.442
3.582   33.645   -1.501
-0.442   -1.501   24.293

orbtensor 7 C
-151.268   -9.725    6.852
-9.725  -182.139   23.501
6.852   23.501  -51.379
239.744   -6.437   -1.437
-6.437   219.976   -4.933
-1.437   -4.933   239.541

orbtensor 8 H
-1.712    5.002   -1.310
5.002    2.058    0.864
-1.310    0.864    2.599
30.478   -6.155    1.280
-6.155   25.719   -0.878
1.280   -0.878   24.297

orbtensor 9 C
-173.461   16.325  -21.442
16.325  -160.753   14.621
-21.442   14.621  -52.730
225.625   11.001    4.222
11.001   234.148   -2.897
4.222   -2.897   239.540

orbtensor 10 H
-1.285   -5.115   -1.158
-5.115    1.558   -0.920
-1.158   -0.920    2.592
29.778    6.378    1.229
6.378   26.397    0.946
1.229    0.946   24.284

orbtensor 11 C

```

-171.675	-17.515	-19.532
-17.515	-163.057	-14.736
-19.532	-14.736	-51.748
226.837	-11.409	4.052
-11.409	232.910	3.121
4.052	3.121	239.521

orbtensor 12 H

4.566	-2.899	-0.377
-2.899	-4.290	-1.414
-0.377	-1.414	2.597
22.540	3.582	0.442
3.582	33.643	1.503
0.442	1.503	24.294

orbtensor 13 C

-151.276	-9.709	-6.809
-9.709	-182.111	-23.475
-6.809	-23.475	-51.321
239.737	-6.437	1.436
-6.437	219.968	4.934
1.436	4.934	239.541

orbtensor 14 H

-1.730	4.992	1.272
4.992	2.043	-0.845
1.272	-0.845	2.533
30.478	-6.154	-1.280
-6.154	25.719	0.878
-1.280	0.878	24.298

orbtensor 15 C

-173.445	16.310	21.441
16.310	-160.763	-14.596
21.441	-14.596	-52.690
225.619	11.002	-4.222
11.002	234.140	2.896
-4.222	2.896	239.538

orbtensor 16 H

-1.311	-5.104	1.110
-5.104	1.539	0.885
1.110	0.885	2.492
29.778	6.378	-1.228
6.378	26.397	-0.946
-1.228	-0.946	24.284

orbtensor 17 C

-171.731	-17.509	19.514
-17.509	-163.080	14.687
19.514	14.687	-51.733
226.834	-11.411	-4.054
-11.411	232.910	-3.120
-4.054	-3.120	239.515

orbtensor 18 H

4.291	3.336	-0.561
3.336	-3.981	1.405
-0.561	1.405	2.595
22.974	-4.168	0.522
-4.168	33.224	-1.472
0.522	-1.472	24.301

orbtensor 19 C

-152.589	10.975	-8.911
10.975	-180.786	23.713
-8.911	23.713	-51.912


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238.988    7.473    1.711
7.473  220.750   -4.849
1.711   -4.849  239.552

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```

orbtensor 20 C
-183.802  -1.288  -25.487
-1.288  -148.802  -0.389
-25.487  -0.389  -52.401
217.970  -0.659   5.117
-0.659  241.639   0.135
5.117    0.135  239.583

```

```

orbtensor 21 H
-5.105   -0.223  -1.539
-0.223   5.523  -0.053
-1.539  -0.053   2.641
34.660   0.361   1.572
0.361   21.472   0.043
1.572    0.043  24.285

```

```

gtensor (ppt)
-0.142   0.000   0.000
0.000  -0.142   0.000
0.000   0.000  -0.131
-12.179  -0.021   0.000
-0.021  -12.203  -0.001
0.000   -0.001  -1.072

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-59.4217	-780.94633	29767.96136	31.73033	29799.69169	29018.74536
2	H	3.1123	27.81033	-410.62256	-0.26601	-410.88857	-383.07824
3	C	-0.8690	104.65133	455.86202	-1.04646	454.81556	559.46689
4	H	3.1447	27.82400	-414.88843	-0.26723	-415.15566	-387.33166
5	C	-0.8707	104.71333	456.73632	-1.03815	455.69817	560.41150
6	H	3.1190	27.79033	-411.50212	-0.26406	-411.76618	-383.97585
7	C	-0.8723	104.82500	457.61063	-1.04162	456.56900	561.39400
8	H	3.0970	27.81300	-408.59958	-0.26847	-408.86804	-381.05504
9	C	-0.8653	104.12300	453.93855	-1.06629	452.87226	556.99526
10	H	3.0957	27.77467	-408.42366	-0.26474	-408.68841	-380.91374
11	C	-0.8663	104.26267	454.46313	-1.06680	453.39633	557.65899
12	H	3.1180	27.78333	-411.37019	-0.26396	-411.63415	-383.85082
13	C	-0.8703	104.84600	456.56146	-1.04297	455.51850	560.36450
14	H	3.0973	27.78033	-408.64355	-0.26843	-408.91199	-381.13165
15	C	-0.8640	104.13300	453.23911	-1.06658	452.17253	556.30553
16	H	3.0957	27.72633	-408.42366	-0.26471	-408.68838	-380.96205
17	C	-0.8663	104.23833	454.46313	-1.06719	453.39594	557.63427
18	H	3.1123	27.80133	-410.62256	-0.26610	-410.88866	-383.08733
19	C	-0.8697	104.66767	456.21174	-1.04576	455.16598	559.83365
20	C	-0.8690	104.72900	455.86202	-1.03943	454.82258	559.55158
21	H	3.1433	27.82533	-414.71252	-0.26730	-414.97982	-387.15449
C Average		-0.8683	104.51893	455.49481	-1.05213	454.44268	558.96162
H Average		3.1135	27.79290	-410.78089	-0.26610	-411.04699	-383.25409

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4VCp2-STO-PBE0-QZ4P-TZ2P
Temperature: 298
Spin: 1.5

```

atensor 1 V
-22.178 -0.001 -0.003
-0.001 -22.161 -0.001
-0.003 -0.001 -79.999
-10.137 0.000 0.000
0.000 -10.133 -0.001
0.000 -0.001 -4.391

atensor 2 H
0.612 -1.365 -1.306
-1.365 3.966 3.676
-1.306 3.676 3.862
0.019 0.007 0.011
0.007 0.002 -0.031
0.003 -0.010 -0.002

atensor 3 C
-1.902 -0.262 -0.599
-0.262 -1.259 1.685
-0.599 1.685 0.010
0.051 0.007 0.009
0.007 0.034 -0.026
0.007 -0.019 0.001

atensor 4 H
4.458 0.119 -3.900
0.119 0.143 -0.107
-3.900 -0.107 3.871
0.000 -0.001 0.032
-0.001 0.022 0.001
0.010 0.000 -0.002

atensor 5 C
-1.167 0.023 -1.787
0.023 -1.997 -0.050
-1.787 -0.050 -0.002
0.031 -0.001 0.028
-0.001 0.054 0.001
0.020 0.001 0.001

atensor 6 H
0.474 1.174 -1.103
1.174 4.107 -3.742
-1.103 -3.742 3.863
0.020 -0.006 0.009
-0.006 0.001 0.031
0.003 0.010 -0.002

atensor 7 C
-1.929 0.225 -0.506
0.225 -1.232 -1.715
-0.506 -1.715 0.009
0.052 -0.006 0.008
-0.006 0.033 0.027
0.006 0.019 0.001

atensor 8 H
3.071 -2.017 3.219
-2.017 1.511 -2.206
3.219 -2.205 3.864
0.007 0.010 -0.027
0.010 0.015 0.018
-0.009 0.006 -0.002

atensor 9 C
-1.432 -0.387 1.474

-0.387 -1.731 -1.011
1.474 -1.011 0.006
0.039 0.010 -0.023
0.010 0.047 0.016
-0.017 0.011 0.001

atensor 10 H
2.847 2.090 3.093
2.090 1.738 2.379
3.093 2.379 3.866
0.008 -0.011 -0.026
-0.011 0.014 -0.020
-0.008 -0.006 -0.002

atensor 11 C
-1.470 0.401 1.418
0.401 -1.683 1.090
1.418 1.090 0.013
0.040 -0.011 -0.022
-0.011 0.045 -0.017
-0.016 -0.012 0.001

atensor 12 H
0.472 1.174 1.103
1.174 4.105 3.742
1.103 3.742 3.863
0.020 -0.006 -0.009
-0.006 0.001 -0.031
-0.003 -0.010 -0.002

atensor 13 C
-1.927 0.225 0.506
0.225 -1.230 1.716
0.506 1.716 0.013
0.052 -0.006 -0.008
-0.006 0.033 -0.027
-0.006 -0.019 0.001

atensor 14 H
3.070 -2.016 -3.219
-2.016 1.510 2.205
-3.219 2.205 3.864
0.007 0.010 0.027
0.010 0.015 -0.018
0.009 -0.006 -0.002

atensor 15 C
-1.431 -0.387 -1.474
-0.387 -1.730 1.011
-1.474 1.011 0.007
0.039 0.010 0.023
0.010 0.047 -0.016
0.017 -0.011 0.001

atensor 16 H
2.847 2.090 -3.093
2.090 1.738 -2.379
-3.092 -2.379 3.865
0.008 -0.011 0.026
-0.011 0.014 0.020
0.008 0.006 -0.002

atensor 17 C
-1.470 0.401 -1.417
0.401 -1.683 -1.091
-1.417 -1.091 0.012
0.040 -0.011 0.022

-0.011 0.045 0.017
0.016 0.012 0.001

atensor 18 H
0.612 -1.365 1.306
-1.365 3.966 -3.676
1.306 -3.676 3.862
0.019 0.007 -0.011
0.007 0.002 0.031
-0.003 0.010 -0.002

atensor 19 C
-1.903 -0.262 0.599
-0.262 -1.260 -1.685
0.599 -1.685 0.008
0.051 0.007 -0.009
0.007 0.034 0.026
-0.007 0.019 0.001

atensor 20 C
-1.167 0.023 1.787
0.023 -1.997 0.049
1.787 0.049 0.000
0.031 -0.001 -0.028
-0.001 0.054 -0.001
-0.020 -0.001 0.001

atensor 21 H
4.457 0.118 3.900
0.118 0.142 0.107
3.900 0.107 3.871
0.000 -0.001 -0.032
-0.001 0.022 -0.001
-0.010 0.000 -0.002

orbtensor 1 V
-3669.854 8.100 -0.029
8.100 -3615.965 -0.223
-0.029 -0.223 -241.431
1704.925 0.000 0.000
0.000 1704.928 -0.001
0.000 -0.001 1721.870

orbtensor 2 H
-1.397 4.497 0.994
4.497 -12.275 -2.504
0.994 -2.504 -0.402
27.519 -4.988 -0.973
-4.988 39.776 2.738
-0.973 2.738 25.210

orbtensor 3 C
-189.054 15.984 7.954
15.984 -227.304 -23.234
7.954 -23.234 -66.905
255.178 2.466 -1.475
2.466 249.131 4.153
-1.475 4.153 233.417

orbtensor 4 H
-14.051 -0.329 2.807
-0.329 0.026 0.033
2.807 0.033 -0.399
41.539 0.434 -2.904
0.434 25.757 -0.080
-2.904 -0.080 25.209

orbtensor 5 C
-233.987 -1.489 24.605
-1.489 -179.920 0.440
24.605 0.440 -66.940
248.269 -0.214 -4.402
-0.214 256.059 -0.120
-4.402 -0.120 233.423

orbtensor 6 H
-0.915 -3.836 0.743
-3.836 -12.751 2.529
0.743 2.529 -0.392
27.009 4.287 -0.822
4.287 40.286 -2.788
-0.822 -2.788 25.209

orbtensor 7 C
-188.184 -13.991 7.312
-13.991 -229.368 23.116
7.312 23.116 -66.675
255.427 -2.119 -1.246
-2.119 248.875 -4.229
-1.246 -4.229 233.414

orbtensor 8 H
-9.516 6.570 -2.347
6.570 -4.378 1.525
-2.347 1.525 -0.406
36.496 -7.371 2.397
-7.371 30.796 -1.643
2.397 -1.643 25.208

orbtensor 9 C
-217.230 24.255 -20.378
24.255 -196.952 14.110
-20.378 14.110 -67.068
250.749 3.639 3.635
3.639 253.564 -2.490
3.635 -2.490 233.418

orbtensor 10 H
-8.828 -6.790 -2.199
-6.790 -5.058 -1.584
-2.199 -1.584 -0.391
35.673 7.638 2.304
7.638 31.620 1.772
2.304 1.772 25.209

orbtensor 11 C
-215.570 -25.137 -19.521
-25.137 -200.582 -14.466
-19.521 -14.466 -66.709
251.158 -3.772 3.492
-3.772 253.159 2.686
3.492 2.686 233.418

orbtensor 12 H
-0.896 -3.842 -0.741
-3.842 -12.742 -2.563
-0.741 -2.563 -0.382
27.009 4.287 0.822
4.287 40.285 2.789
0.822 2.789 25.210

orbtensor 13 C
-188.167 -13.994 -7.315
-13.994 -229.351 -23.156

-7.315 -23.156 -66.693
255.428 -2.118 1.246
-2.118 248.875 4.229
1.246 4.229 233.413

orbtensor 14 H
-9.512 6.571 2.363
6.571 -4.374 -1.530
2.363 -1.530 -0.401
36.496 -7.371 -2.398
-7.371 30.796 1.643
-2.398 1.643 25.208

orbtensor 15 C
-217.225 24.267 20.397
24.267 -196.960 -14.139
20.397 -14.139 -67.073
250.745 3.640 -3.634
3.640 253.566 2.492
-3.634 2.492 233.416

orbtensor 16 H
-8.814 -6.799 2.230
-6.799 -5.047 1.597
2.230 1.597 -0.374
35.674 7.638 -2.303
7.638 31.621 -1.771
-2.303 -1.771 25.209

orbtensor 17 C
-215.585 -25.147 19.542
-25.147 -200.577 14.456
19.542 14.456 -66.704
251.162 -3.772 -3.493
-3.772 253.160 -2.683
-3.493 -2.683 233.420

orbtensor 18 H
-1.383 4.496 -1.021
4.496 -12.273 2.516
-1.021 2.516 -0.394
27.518 -4.988 0.973
-4.988 39.777 -2.737
0.973 -2.737 25.209

orbtensor 19 C
-189.048 15.989 -7.985
15.989 -227.325 23.230
-7.985 23.230 -66.911
255.178 2.466 1.476
2.466 249.131 -4.151
1.476 -4.151 233.415

orbtensor 20 C
-234.003 -1.490 -24.632
-1.490 -179.920 -0.444
-24.632 -0.444 -66.954
248.270 -0.214 4.402
-0.214 256.060 0.123
4.402 0.123 233.423

orbtensor 21 H
-14.046 -0.333 -2.830
-0.333 0.037 -0.021
-2.830 -0.021 -0.391
41.539 0.433 2.904
0.433 25.757 0.080

2.904 0.080 25.209

gtensor (ppt)

-0.147 0.000 0.000
0.000 -0.147 0.000
0.000 0.000 -0.129
-11.394 -0.055 0.000
-0.055 -11.773 -0.001
0.000 -0.001 -0.891

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	V	-49.6663	-798.50900	24886.68989	31.15042	24917.84031	24119.33131
2	H	2.8197	26.14367	-372.09621	-0.23497	-372.33118	-346.18752
3	C	-1.0217	84.82100	536.07262	-0.96183	535.11079	619.93179
4	H	2.8307	26.02700	-373.54782	-0.26298	-373.81080	-347.78380
5	C	-1.0267	85.63467	538.69614	-0.97670	537.71944	623.35411
6	H	2.8210	26.14867	-372.27217	-0.22793	-372.50010	-346.35143
7	C	-1.0220	84.49633	536.24752	-0.95636	535.29117	619.78750
8	H	2.8220	26.06667	-372.40413	-0.25716	-372.66129	-346.59463
9	C	-1.0233	85.49367	536.94713	-0.97653	535.97060	621.46427
10	H	2.8237	26.07500	-372.62407	-0.24525	-372.86932	-346.79432
11	C	-1.0180	84.95800	534.14871	-0.96895	533.17976	618.13776
12	H	2.8197	26.16133	-372.09621	-0.22792	-372.32413	-346.16280
13	C	-1.0193	84.50167	534.84831	-0.95702	533.89130	618.39296
14	H	2.8213	26.07100	-372.31615	-0.25712	-372.57328	-346.50228
15	C	-1.0223	85.48967	536.42243	-0.97618	535.44625	620.93592
16	H	2.8233	26.08967	-372.58008	-0.24530	-372.82538	-346.73572
17	C	-1.0183	84.95867	534.32361	-0.96870	533.35491	618.31358
18	H	2.8197	26.15133	-372.09621	-0.23529	-372.33151	-346.18017
19	C	-1.0230	84.81333	536.77223	-0.96179	535.81044	620.62377
20	C	-1.0260	85.62533	538.34634	-0.97794	537.36840	622.99374
21	H	2.8300	26.03500	-373.45985	-0.26313	-373.72298	-347.68798
	C Average	-1.0221	85.07923	536.28251	-0.96820	535.31430	620.39354
	H Average	2.8231	26.09693	-372.54929	-0.24571	-372.79500	-346.69806

4VCp2-STO-PBE0-QZ4P-QZ4P

Temperature: 298

Spin: 1.5

atensor 1 V

-18.077 -0.001 -0.001
-0.001 -18.060 -0.001
-0.001 -0.001 -76.436
-10.079 -0.001 0.000
-0.001 -10.075 -0.001
0.000 -0.001 -4.388

atensor 2 H

0.584 -1.358 -1.307
-1.358 3.921 3.679
-1.307 3.679 3.872
0.020 0.007 0.011
0.007 0.003 -0.030
0.003 -0.010 -0.002

atensor 3 C

-2.059 -0.256 -0.596
-0.256 -1.430 1.677
-0.596 1.677 -0.207
0.052 0.007 0.009
0.007 0.035 -0.026
0.007 -0.019 0.001

atensor 4 H
4.408 0.118 -3.903
0.118 0.116 -0.108
-3.903 -0.108 3.878
0.000 -0.001 0.032
-0.001 0.022 0.001
0.010 0.000 -0.002

atensor 5 C
-1.343 0.022 -1.778
0.022 -2.155 -0.049
-1.778 -0.049 -0.221
0.032 -0.001 0.028
-0.001 0.054 0.001
0.021 0.001 0.001

atensor 6 H
0.447 1.168 -1.104
1.168 4.061 -3.745
-1.104 -3.745 3.873
0.020 -0.006 0.009
-0.006 0.002 0.031
0.003 0.010 -0.002

atensor 7 C
-2.086 0.220 -0.503
0.220 -1.404 -1.708
-0.503 -1.708 -0.208
0.053 -0.006 0.008
-0.006 0.034 0.027
0.006 0.020 0.001

atensor 8 H
3.028 -2.006 3.221
-2.006 1.476 -2.207
3.221 -2.207 3.870
0.007 0.010 -0.026
0.010 0.015 0.018
-0.008 0.006 -0.002

atensor 9 C
-1.600 -0.379 1.467
-0.379 -1.893 -1.006
1.467 -1.006 -0.211
0.039 0.010 -0.023
0.010 0.047 0.016
-0.017 0.012 0.001

atensor 10 H
2.806 2.079 3.095
2.079 1.702 2.381
3.095 2.381 3.873
0.008 -0.010 -0.025
-0.010 0.014 -0.019
-0.008 -0.006 -0.002

atensor 11 C
-1.640 0.393 1.411
0.393 -1.849 1.085
1.411 1.085 -0.207

0.041 -0.011 -0.022
-0.011 0.046 -0.017
-0.016 -0.013 0.001

atensor 12 H
0.446 1.168 1.104
1.168 4.060 3.745
1.104 3.745 3.873
0.020 -0.006 -0.009
-0.006 0.002 -0.031
-0.003 -0.010 -0.002

atensor 13 C
-2.085 0.220 0.503
0.220 -1.403 1.708
0.503 1.708 -0.205
0.053 -0.006 -0.008
-0.006 0.034 -0.027
-0.006 -0.020 0.001

atensor 14 H
3.027 -2.006 -3.221
-2.006 1.475 2.207
-3.221 2.207 3.870
0.007 0.010 0.026
0.010 0.015 -0.018
0.008 -0.006 -0.002

atensor 15 C
-1.600 -0.379 -1.467
-0.379 -1.893 1.006
-1.467 1.006 -0.211
0.039 0.010 0.023
0.010 0.047 -0.016
0.017 -0.012 0.001

atensor 16 H
2.806 2.079 -3.095
2.079 1.703 -2.381
-3.095 -2.381 3.872
0.008 -0.010 0.025
-0.010 0.014 0.019
0.008 0.006 -0.002

atensor 17 C
-1.641 0.393 -1.410
0.393 -1.849 -1.086
-1.410 -1.086 -0.209
0.041 -0.011 0.022
-0.011 0.046 0.017
0.016 0.013 0.001

atensor 18 H
0.585 -1.358 1.307
-1.358 3.922 -3.679
1.307 -3.679 3.872
0.020 0.007 -0.011
0.007 0.003 0.030
-0.003 0.010 -0.002

atensor 19 C
-2.060 -0.256 0.596
-0.256 -1.431 -1.677
0.596 -1.677 -0.209
0.052 0.007 -0.009
0.007 0.035 0.026
-0.007 0.019 0.001

atensor 20 C
-1.342 0.022 1.778
0.022 -2.154 0.049
1.778 0.049 -0.219
0.032 -0.001 -0.028
-0.001 0.054 -0.001
-0.021 -0.001 0.001

atensor 21 H
4.408 0.118 3.903
0.118 0.115 0.107
3.903 0.107 3.878
0.000 -0.001 -0.032
-0.001 0.022 -0.001
-0.010 0.000 -0.002

orbtensor 1 V
-3604.080 5.030 -0.026
5.030 -3594.033 -0.265
-0.026 -0.265 -246.790
1696.226 0.000 0.000
0.000 1696.230 0.000
0.000 0.000 1726.330

orbtensor 2 H
1.247 5.582 0.813
5.582 -12.409 -2.107
0.813 -2.107 1.438
24.577 -6.148 -0.715
-6.148 39.685 2.009
-0.715 2.009 23.070

orbtensor 3 C
-189.324 18.199 8.623
18.199 -237.134 -21.287
8.623 -21.287 -70.437
251.795 -0.055 -1.316
-0.055 251.937 3.704
-1.316 3.704 230.749

orbtensor 4 H
-14.490 -0.451 2.292
-0.451 3.160 0.005
2.292 0.005 1.440
41.857 0.534 -2.131
0.534 22.407 -0.059
-2.131 -0.059 23.068

orbtensor 5 C
-244.860 -3.161 22.621
-3.161 -183.209 -0.316
22.621 -0.316 -70.445
251.965 0.005 -3.927
0.005 251.787 -0.107
-3.927 -0.107 230.755

orbtensor 6 H
1.741 -4.732 0.565
-4.732 -13.039 2.107
0.565 2.107 1.441
23.949 5.284 -0.603
5.284 40.313 -2.045
-0.603 -2.045 23.069

orbtensor 7 C
-186.791 -18.856 6.505

-18.856	-238.309	21.292
6.505	21.292	-70.432
251.787	0.047	-1.111
0.047	251.940	-3.769
-1.111	-3.769	230.746

orbtensor 8 H

-8.838	8.221	-1.888
8.221	-2.456	1.272
-1.888	1.272	1.442
35.642	-9.085	1.760
-9.085	28.616	-1.206
1.760	-1.206	23.068

orbtensor 9 C

-225.106	28.735	-20.191
28.735	-202.874	14.129
-20.191	14.129	-70.432
251.899	-0.085	3.243
-0.085	251.834	-2.221
3.243	-2.221	230.751

orbtensor 10 H

-8.028	-8.463	-1.781
-8.463	-3.425	-1.281
-1.781	-1.281	1.443
34.627	9.414	1.692
9.414	29.632	1.301
1.692	1.301	23.068

orbtensor 11 C

-220.079	-32.236	-17.626
-32.236	-205.941	-13.795
-17.626	-13.795	-70.458
251.887	0.088	3.116
0.088	251.842	2.397
3.116	2.397	230.751

orbtensor 12 H

1.739	-4.731	-0.566
-4.731	-13.040	-2.104
-0.566	-2.104	1.438
23.950	5.283	0.604
5.283	40.313	2.046
0.604	2.046	23.070

orbtensor 13 C

-186.784	-18.854	-6.507
-18.854	-238.306	-21.315
-6.507	-21.315	-70.437
251.788	0.047	1.111
0.047	251.941	3.772
1.111	3.772	230.748

orbtensor 14 H

-8.838	8.220	1.889
8.220	-2.456	-1.270
1.889	-1.270	1.440
35.644	-9.084	-1.760
-9.084	28.616	1.206
-1.760	1.206	23.069

orbtensor 15 C

-225.113	28.727	20.193
28.727	-202.872	-14.137
20.193	-14.137	-70.440
251.905	-0.084	-3.242

-0.084 251.834 2.223
-3.242 2.223 230.756

orbtensor 16 H
-8.026 -8.462 1.782
-8.462 -3.425 1.280
1.782 1.280 1.443
34.627 9.415 -1.690
9.415 29.632 -1.300
-1.690 -1.300 23.067

orbtensor 17 C
-220.053 -32.235 17.618
-32.235 -205.935 13.781
17.618 13.781 -70.459
251.887 0.088 -3.116
0.088 251.841 -2.394
-3.116 -2.394 230.748

orbtensor 18 H
1.247 5.583 -0.813
5.583 -12.410 2.101
-0.813 2.101 1.438
24.577 -6.148 0.714
-6.148 39.685 -2.007
0.714 -2.007 23.069

orbtensor 19 C
-189.315 18.203 -8.619
18.203 -237.135 21.274
-8.619 21.274 -70.426
251.796 -0.055 1.316
-0.055 251.938 -3.701
1.316 -3.701 230.749

orbtensor 20 C
-244.850 -3.165 -22.631
-3.165 -183.199 0.305
-22.631 0.305 -70.438
251.965 0.005 3.928
0.005 251.787 0.110
3.928 0.110 230.755

orbtensor 21 H
-14.489 -0.451 -2.292
-0.451 3.158 -0.007
-2.292 -0.007 1.439
41.857 0.534 2.131
0.534 22.408 0.059
2.131 0.059 23.068

gtensor (ppt)
-0.150 0.000 0.000
0.000 -0.150 0.000
0.000 0.000 -0.124
-11.430 0.003 0.000
0.003 -11.453 -0.001
0.000 -0.001 -0.896

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
---	----	------------	---------------	-----------	-----------	--------------	---------

1	V	-45.7050	-775.37233	22902.81849	31.09589	22933.91439	22158.54205
2	H	2.7993	25.86933	-369.43010	-0.24849	-369.67859	-343.80925
3	C	-1.2027	79.19533	631.07338	-0.92306	630.15031	709.34565
4	H	2.8073	25.81400	-370.48586	-0.25031	-370.73617	-344.92217
5	C	-1.2107	78.66433	635.27121	-0.91936	634.35185	713.01618
6	H	2.8003	25.82467	-369.56207	-0.24908	-369.81115	-343.98648
7	C	-1.2033	79.64700	631.42320	-0.92353	630.49966	710.14666
8	H	2.7980	25.82467	-369.25414	-0.24974	-369.50388	-343.67921
9	C	-1.2057	78.69067	632.64756	-0.92344	631.72412	710.41479
10	H	2.8003	25.77233	-369.56207	-0.25012	-369.81219	-344.03985
11	C	-1.2027	79.33400	631.07338	-0.92432	630.14906	709.48306
12	H	2.7997	25.82333	-369.47409	-0.24890	-369.72299	-343.89966
13	C	-1.2017	79.65000	630.54865	-0.92418	629.62447	709.27447
14	H	2.7973	25.82500	-369.16616	-0.24970	-369.41586	-343.59086
15	C	-1.2057	78.69000	632.64756	-0.92309	631.72447	710.41447
16	H	2.8003	25.77267	-369.56207	-0.25009	-369.81216	-344.03950
17	C	-1.2037	79.34300	631.59811	-0.92377	630.67434	710.01734
18	H	2.8000	25.86867	-369.51808	-0.24866	-369.76673	-343.89807
19	C	-1.2040	79.20233	631.77302	-0.92303	630.84999	710.05232
20	C	-1.2093	78.67333	634.57157	-0.91996	633.65161	712.32494
21	H	2.8070	25.81367	-370.44187	-0.25038	-370.69225	-344.87858
C Average		-1.2049	79.10900	632.26276	-0.92277	631.33999	710.44899
H Average		2.8010	25.82083	-369.64565	-0.24955	-369.89520	-344.07436

6MnCp2-STO-PBE0-DZ-DZ

Temperature: 390

Spin: 2.5

atensor 1 Mn

-104.839 -0.004 -0.002
-0.004 -104.826 -0.002
-0.002 -0.002 -100.212
-2.428 0.000 0.000
0.000 -2.428 0.000
0.000 0.000 -2.843

atensor 2 H

-2.413 -1.463 -1.231
-1.463 1.181 3.462
-1.231 3.462 0.662
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

atensor 3 C

-0.214 -0.279 -0.635
-0.279 0.469 1.782
-0.635 1.782 3.774
0.001 -0.001 -0.001
-0.001 0.004 0.002
0.001 -0.002 0.000

atensor 4 H

1.707 0.127 -3.672
0.127 -2.919 -0.100
-3.672 -0.100 0.674
0.001 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C

0.578 0.024 -1.895
0.024 -0.303 -0.052

-1.895 -0.052 3.789
0.004 0.000 -0.002
0.000 0.001 0.000
0.002 0.000 0.000

atensor 6 H
-2.557 1.257 -1.040
1.257 1.335 -3.524
-1.040 -3.524 0.668
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 7 C
-0.242 0.240 -0.538
0.240 0.497 -1.814
-0.538 -1.814 3.773
0.001 0.001 0.000
0.001 0.004 -0.002
0.001 0.002 0.000

atensor 8 H
0.211 -2.163 3.031
-2.163 -1.460 -2.078
3.031 -2.078 0.654
0.000 -0.001 0.001
-0.001 0.000 -0.001
0.000 0.000 0.000

atensor 9 C
0.289 -0.411 1.563
-0.411 -0.030 -1.069
1.563 -1.069 3.778
0.003 -0.002 0.001
-0.002 0.002 -0.001
-0.002 0.001 0.000

atensor 10 H
-0.031 2.241 2.912
2.241 -1.219 2.240
2.912 2.240 0.654
0.000 0.001 0.001
0.001 0.000 0.001
0.000 0.000 0.000

atensor 11 C
0.244 0.426 1.502
0.426 0.017 1.154
1.502 1.154 3.781
0.003 0.002 0.001
0.002 0.002 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.557 1.257 1.039
1.257 1.335 3.525
1.039 3.525 0.669
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

atensor 13 C
-0.242 0.240 0.537
0.240 0.497 1.814
0.537 1.814 3.773
0.001 0.001 0.000
0.001 0.004 0.002

-0.001 -0.002 0.000

atensor 14 H
0.209 -2.162 -3.031
-2.162 -1.464 2.076
-3.031 2.076 0.652
0.000 -0.001 -0.001
-0.001 0.000 0.001
0.000 0.000 0.000

atensor 15 C
0.290 -0.411 -1.563
-0.411 -0.030 1.068
-1.563 1.068 3.782
0.003 -0.002 -0.001
-0.002 0.002 0.001
0.002 -0.001 0.000

atensor 16 H
-0.034 2.241 -2.911
2.241 -1.220 -2.240
-2.911 -2.240 0.651
0.000 0.001 -0.001
0.001 0.000 -0.001
0.000 0.000 0.000

atensor 17 C
0.245 0.426 -1.502
0.426 0.018 -1.154
-1.502 -1.154 3.784
0.003 0.002 -0.001
0.002 0.002 -0.001
0.002 0.001 0.000

atensor 18 H
-2.412 -1.463 1.231
-1.463 1.183 -3.462
1.231 -3.462 0.663
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 19 C
-0.215 -0.279 0.635
-0.279 0.468 -1.782
0.635 -1.782 3.771
0.001 -0.001 0.001
-0.001 0.004 -0.002
-0.001 0.002 0.000

atensor 20 C
0.577 0.024 1.896
0.024 -0.304 0.052
1.896 0.052 3.784
0.004 0.000 0.002
0.000 0.001 0.000
-0.002 0.000 0.000

atensor 21 H
1.711 0.127 3.673
0.127 -2.915 0.101
3.673 0.101 0.678
0.001 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn

```
-1645.028   -5.874    0.200
-5.874 -1691.732   -0.073
0.200   -0.073  -109.273
1934.519   -0.001    0.001
-0.001  1934.522    0.000
0.001    0.000  1940.517
```

```
orbtensor 2 H
1.340    5.399    0.599
5.399  -12.193   -1.899
0.599   -1.899    3.060
25.170   -5.605   -0.928
-5.605   38.962    2.610
-0.928    2.610   24.008
```

```
orbtensor 3 C
-186.045   12.344    3.791
12.344  -221.078   -17.138
3.791   -17.138  -56.804
261.634    7.073   -0.600
7.073  244.333    1.708
-0.600    1.708   242.230
```

```
orbtensor 4 H
-14.057   -0.527    2.023
-0.527    3.242    0.092
2.023    0.092    3.072
40.916    0.486   -2.768
0.486   23.185   -0.076
-2.768   -0.076   24.000
```

```
orbtensor 5 C
-225.318   -1.575   17.595
-1.575  -181.924    3.059
17.595    3.059  -56.760
241.739   -0.616   -1.789
-0.616  264.153   -0.047
-1.789   -0.047  242.218
```

```
orbtensor 6 H
1.858   -4.734    0.645
-4.734  -12.794    1.949
0.645    1.949    2.955
24.591    4.819   -0.784
4.819   39.526   -2.658
-0.784   -2.658   24.001
```

```
orbtensor 7 C
-186.185  -10.757    6.332
-10.757  -223.835   17.085
6.332   17.085  -54.689
262.334   -6.091   -0.504
-6.091  243.584   -1.737
-0.504   -1.737  242.209
```

```
orbtensor 8 H
-8.488    8.078   -1.539
8.078   -2.347    1.091
-1.539    1.091    2.849
35.262   -8.290    2.280
-8.290   28.852   -1.564
2.280   -1.564   23.997
```

```
orbtensor 9 C
-209.492   21.006  -14.121
21.006  -196.993    9.456
-14.121    9.456  -55.526
```


248.945	10.419	1.489
10.419	257.010	-1.018
1.489	-1.018	242.213

orbtensor 10 H

-7.639	-8.469	-1.583
-8.469	-3.300	-1.330
-1.583	-1.330	2.934
34.330	8.590	2.190
8.590	29.768	1.685
2.190	1.685	23.987

orbtensor 11 C

-209.242	-21.600	-13.764
-21.600	-201.526	-12.216
-13.764	-12.216	-54.807
250.103	-10.803	1.427
-10.803	255.846	1.097
1.427	1.097	242.193

orbtensor 12 H

1.861	-4.730	-0.645
-4.730	-12.795	-1.952
-0.645	-1.952	2.960
24.588	4.815	0.783
4.815	39.527	2.659
0.783	2.659	24.001

orbtensor 13 C

-186.175	-10.738	-6.296
-10.738	-223.848	-17.071
-6.296	-17.071	-54.801
262.331	-6.092	0.497
-6.092	243.583	1.737
0.497	1.737	242.210

orbtensor 14 H

-8.493	8.078	1.543
8.078	-2.345	-1.094
1.543	-1.094	2.851
35.267	-8.289	-2.283
-8.289	28.850	1.565
-2.283	1.565	23.998

orbtensor 15 C

-209.533	21.008	14.138
21.008	-197.012	-9.456
14.138	-9.456	-55.625
248.952	10.416	-1.491
10.416	257.019	1.017
-1.491	1.017	242.213

orbtensor 16 H

-7.637	-8.471	1.584
-8.471	-3.304	1.332
1.584	1.332	2.940
34.328	8.591	-2.190
8.591	29.771	-1.685
-2.190	-1.685	23.986

orbtensor 17 C

-209.273	-21.609	13.765
-21.609	-201.549	12.168
13.765	12.168	-54.919
250.112	-10.803	-1.431
-10.803	255.850	-1.092
-1.431	-1.092	242.192

```

orbtensor 18 H
1.341    5.400   -0.601
5.400   -12.189    1.900
-0.601    1.900    3.067
25.171   -5.607    0.927
-5.607   38.961   -2.607
0.927    -2.607   24.007

```

```

orbtensor 19 C
-186.041  12.334   -3.760
12.334  -221.062   17.085
-3.760   17.085  -56.940
261.625    7.080    0.595
7.080   244.332   -1.709
0.595   -1.709   242.225

```

```

orbtensor 20 C
-225.299  -1.574   -17.538
-1.574  -181.901   -3.075
-17.538  -3.075  -56.886
241.732   -0.621    1.790
-0.621   264.145    0.049
1.790    0.049   242.223

```

```

orbtensor 21 H
-14.055   -0.529   -2.024
-0.529    3.242   -0.092
-2.024   -0.092    3.078
40.915    0.488    2.767
0.488   23.185    0.076
2.767    0.076   24.001

```

```

gtensor (ppt)
-0.141    0.000    0.000
0.000   -0.141    0.000
0.000    0.000   -0.162
0.152    0.014    0.000
0.014    0.302    0.000
0.000    0.000    0.052

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-105.8587	787.84167	100679.54797	0.08687	100679.63484	101467.47651
2	H	-0.1897	26.78233	44.80794	-0.00243	44.80551	71.58785
3	C	1.3447	94.75667	-1263.09358	0.06764	-1263.02594	-1168.26927
4	H	-0.1790	26.78600	42.28799	0.02008	42.30807	69.09407
5	C	1.3563	94.70267	-1274.05250	0.08482	-1273.96767	-1179.26501
6	H	-0.1843	26.71233	43.54796	-0.00630	43.54167	70.25400
7	C	1.3443	94.47267	-1262.78047	0.06468	-1262.71579	-1168.24312
8	H	-0.1983	26.70833	46.85540	0.01388	46.86928	73.57762
9	C	1.3473	95.38567	-1265.59847	0.08006	-1265.51841	-1170.13275
10	H	-0.1987	26.69333	46.93415	0.00761	46.94176	73.63509
11	C	1.3490	94.18900	-1267.16403	0.07534	-1267.08869	-1172.89969
12	H	-0.1840	26.71400	43.46921	-0.00629	43.46292	70.17692
13	C	1.3443	94.43333	-1262.78047	0.06468	-1262.71579	-1168.28245
14	H	-0.2010	26.70933	47.48539	0.01389	47.49928	74.20862
15	C	1.3490	95.33800	-1267.16403	0.08014	-1267.08389	-1171.74589
16	H	-0.2010	26.69467	47.48539	0.00760	47.49299	74.18765
17	C	1.3507	94.13767	-1268.72959	0.07538	-1268.65421	-1174.51655

18	H	-0.1883	26.78600	44.49295	-0.00243	44.49051	71.27651
19	C	1.3430	94.71300	-1261.52802	0.06760	-1261.46042	-1166.74742
20	C	1.3540	94.67133	-1271.86071	0.08474	-1271.77597	-1177.10464
21	H	-0.1750	26.78867	41.34300	0.02008	41.36309	68.15175
C Average		1.3483	94.68000	-1266.47519	0.07451	-1266.40068	-1171.72068
H Average		-0.1899	26.73750	44.87094	0.00657	44.87751	71.61501

=====
6MnCp2-STO-PBE0-DZ-TZ2P
Temperature: 390
Spin: 2.5

atensor 1 Mn
-101.205 0.000 -0.002
0.000 -101.218 -0.001
-0.002 -0.001 -96.953
-2.542 0.000 0.000
0.000 -2.541 0.000
0.000 0.000 -2.883

atensor 2 H
-2.345 -1.451 -1.217
-1.451 1.221 3.423
-1.217 3.423 0.876
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
-0.029 -0.262 -0.632
-0.262 0.616 1.779
-0.632 1.779 3.978
0.000 -0.001 0.000
-0.001 0.003 0.001
0.001 -0.002 0.000

atensor 4 H
1.736 0.126 -3.631
0.126 -2.853 -0.099
-3.631 -0.099 0.880
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.708 0.023 -1.887
0.023 -0.122 -0.051
-1.887 -0.051 3.981
0.004 0.000 -0.001
0.000 0.000 0.000
0.002 0.000 0.000

atensor 6 H
-2.491 1.247 -1.028
1.247 1.370 -3.485
-1.028 -3.485 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
-0.056 0.225 -0.534
0.225 0.643 -1.811
-0.534 -1.811 3.976
0.000 0.001 0.000

0.001 0.003 -0.001
0.001 0.002 0.000

atensor 8 H
0.269 -2.144 2.998
-2.144 -1.389 -2.055
2.998 -2.055 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.445 -0.388 1.557
-0.388 0.146 -1.067
1.557 -1.067 3.980
0.002 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.029 2.222 2.881
2.222 -1.150 2.216
2.881 2.216 0.878
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.405 0.402 1.496
0.402 0.192 1.151
1.496 1.151 3.983
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.491 1.247 1.027
1.247 1.371 3.486
1.027 3.486 0.880
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
-0.056 0.225 0.533
0.225 0.642 1.811
0.533 1.811 3.976
0.000 0.001 0.000
0.001 0.003 0.001
-0.001 -0.002 0.000

atensor 14 H
0.267 -2.144 -2.998
-2.144 -1.392 2.053
-2.998 2.053 0.877
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.446 -0.387 -1.557
-0.387 0.146 1.066
-1.557 1.066 3.983
0.002 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.027 2.222 -2.879
2.222 -1.151 -2.216
-2.879 -2.216 0.875
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.406 0.402 -1.496
0.402 0.193 -1.151
-1.496 -1.151 3.987
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.001 0.000

atensor 18 H
-2.344 -1.451 1.217
-1.451 1.222 -3.424
1.217 -3.424 0.876
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.030 -0.263 0.632
-0.263 0.616 -1.779
0.632 -1.779 3.975
0.000 -0.001 0.000
-0.001 0.003 -0.001
-0.001 0.002 0.000

atensor 20 C
0.707 0.022 1.887
0.022 -0.123 0.051
1.887 0.051 3.976
0.004 0.000 0.001
0.000 0.000 0.000
-0.002 0.000 0.000

atensor 21 H
1.739 0.126 3.632
0.126 -2.850 0.099
3.632 0.099 0.883
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-1701.008 -19.601 0.200
-19.601 -1694.445 -0.090
0.200 -0.090 -128.618
1938.459 0.000 0.001
0.000 1938.458 0.000
0.001 0.000 1940.199

orbtensor 2 H
-1.459 5.379 1.151
5.379 -14.688 -3.302
1.151 -3.302 -0.318
27.225 -4.783 -1.156
-4.783 38.985 3.252
-1.156 3.252 25.104

orbtensor 3 C
-206.004 14.772 5.694
14.772 -242.885 -15.751

5.694	-15.751	-64.595
251.143	2.779	-1.805
2.779	244.321	5.077
-1.805	5.077	232.253

orbtensor 4 H

-16.741	-0.484	3.516
-0.484	0.362	0.109
3.516	0.109	-0.412
40.672	0.415	-3.451
0.415	25.535	-0.094
-3.451	-0.094	25.101

orbtensor 5 C

-250.506	-0.877	16.833
-0.877	-200.985	0.665
16.833	0.665	-64.707
243.342	-0.240	-5.386
-0.240	252.136	-0.146
-5.386	-0.146	232.259

orbtensor 6 H

-0.886	-4.613	0.927
-4.613	-15.179	3.290
0.927	3.290	-0.400
26.737	4.113	-0.977
4.113	39.471	-3.311
-0.977	-3.311	25.103

orbtensor 7 C

-205.331	-12.629	4.805
-12.629	-243.123	15.772
4.805	15.772	-64.953
251.425	-2.390	-1.526
-2.390	244.033	-5.167
-1.526	-5.167	232.254

orbtensor 8 H

-11.253	7.987	-2.950
7.987	-5.071	1.988
-2.950	1.988	-0.308
35.834	-7.070	2.848
-7.070	30.367	-1.952
2.848	-1.952	25.101

orbtensor 9 C

-234.101	23.312	-14.245
23.312	-216.675	9.317
-14.245	9.317	-64.461
246.137	4.106	4.447
4.106	249.311	-3.047
4.447	-3.047	232.257

orbtensor 10 H

-10.278	-8.247	-2.805
-8.247	-5.935	-2.147
-2.805	-2.147	-0.255
35.047	7.326	2.737
7.326	31.157	2.105
2.737	2.105	25.102

orbtensor 11 C

-231.553	-22.516	-13.257
-22.516	-218.519	-10.036
-13.257	-10.036	-64.768
246.595	-4.254	4.273
-4.254	248.857	3.287

```

4.273      3.287      232.255

orbtensor 12 H
-0.875     -4.612     -0.950
-4.612    -15.184    -3.277
-0.950     -3.277    -0.379
26.735     4.110     0.976
4.110     39.471     3.313
0.976      3.313     25.104

orbtensor 13 C
-205.314   -12.610    -4.769
-12.610   -243.149   -15.782
-4.769    -15.782   -64.962
251.423    -2.390     1.517
-2.390    244.031     5.170
1.517      5.170    232.257

orbtensor 14 H
-11.265     7.989      2.932
7.989     -5.068     -2.002
2.932     -2.002     -0.331
35.837    -7.069     -2.850
-7.069    30.366      1.952
-2.850     1.952     25.101

orbtensor 15 C
-234.184    23.328    14.287
23.328   -216.714    -9.361
14.287    -9.361   -64.516
246.142     4.105    -4.450
4.105    249.319     3.046
-4.450     3.046    232.255

orbtensor 16 H
-10.278    -8.255      2.800
-8.255    -5.939      2.126
2.800      2.126    -0.261
35.045     7.327    -2.737
7.327    31.160    -2.105
-2.737    -2.105     25.101

orbtensor 17 C
-231.602   -22.532    13.311
-22.532  -218.546     9.986
13.311     9.986   -64.799
246.602    -4.254    -4.276
-4.254    248.860    -3.283
-4.276    -3.283    232.252

orbtensor 18 H
-1.455      5.381     -1.146
5.381   -14.689     3.307
-1.146      3.307    -0.293
27.227    -4.784     1.155
-4.784    38.984    -3.250
1.155     -3.250     25.104

orbtensor 19 C
-205.984    14.769    -5.629
14.769  -242.894    15.732
-5.629    15.732   -64.590
251.139     2.781     1.800
2.781    244.322    -5.076
1.800    -5.076    232.251

orbtensor 20 C

```

```

-250.490   -0.879   -16.777
-0.879  -200.953   -0.664
-16.777   -0.664   -64.692
243.334   -0.243    5.383
-0.243   252.126    0.150
5.383     0.150   232.259

```

```

orbtensor 21 H
-16.742   -0.489   -3.517
-0.489    0.366   -0.087
-3.517   -0.087   -0.372
40.671    0.416    3.449
0.416    25.535    0.095
3.449     0.095    25.102

```

```

gtensor (ppt)
-0.142    0.000    0.000
0.000   -0.142    0.000
0.000    0.000   -0.160
-0.018    0.058    0.000
0.058   -0.066    0.000
0.000    0.000   -0.030

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-102.4473	764.34833	97425.05706	0.00244	97425.05950	98189.40783
2	H	-0.0827	24.94967	19.52763	0.01021	19.53784	44.48751
3	C	1.5227	71.41100	-1430.14773	0.00951	-1430.13822	-1358.72722
4	H	-0.0790	24.83900	18.66149	-0.00468	18.65681	43.49581
5	C	1.5237	70.51300	-1431.08697	-0.00124	-1431.08821	-1360.57521
6	H	-0.0807	24.94867	19.05519	-0.00182	19.05337	44.00204
7	C	1.5220	71.43500	-1429.52157	0.00084	-1429.52073	-1358.08573
8	H	-0.0803	24.89000	18.97645	0.00844	18.98489	43.87489
9	C	1.5247	70.82267	-1432.02621	0.00825	-1432.01796	-1361.19529
10	H	-0.0810	24.94600	19.13393	-0.01102	19.12291	44.06891
11	C	1.5277	70.95567	-1434.84392	-0.00583	-1434.84975	-1363.89409
12	H	-0.0800	24.95733	18.89771	-0.00182	18.89589	43.85322
13	C	1.5217	71.42867	-1429.20849	0.00083	-1429.20766	-1357.77899
14	H	-0.0827	24.88000	19.52763	0.00844	19.53607	44.41607
15	C	1.5260	70.76733	-1433.27853	0.00823	-1433.27029	-1362.50296
16	H	-0.0830	24.94267	19.60637	-0.01102	19.59535	44.53802
17	C	1.5297	70.92233	-1436.72240	-0.00583	-1436.72823	-1365.80589
18	H	-0.0820	24.95933	19.37015	0.01021	19.38036	44.33970
19	C	1.5213	71.41467	-1428.89541	0.00953	-1428.88588	-1357.47122
20	C	1.5213	70.52800	-1428.89541	-0.00123	-1428.89664	-1358.36864
21	H	-0.0760	24.85333	17.95282	-0.00468	17.94814	42.80148
C Average		1.5241	71.01983	-1431.46266	0.00231	-1431.46036	-1360.44052
H Average		-0.0807	24.91660	19.07094	0.00023	19.07116	43.98776

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=====
6MnCp2-STO-PBE0-DZ-QZ4P
Temperature: 390
Spin: 2.5

```

```

atensor 1 Mn
-99.667 -0.001 -0.002
-0.001 -99.679 -0.001
-0.002 -0.001 -95.692

```


-2.578 0.000 0.000
0.000 -2.578 0.000
0.000 0.000 -2.884

atensor 2 H
-2.314 -1.445 -1.215
-1.445 1.238 3.419
-1.215 3.419 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
-0.172 -0.261 -0.633
-0.261 0.470 1.783
-0.633 1.783 3.844
0.000 -0.001 0.000
-0.001 0.003 0.001
0.001 -0.002 0.000

atensor 4 H
1.751 0.125 -3.627
0.125 -2.822 -0.099
-3.627 -0.099 0.883
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.562 0.023 -1.891
0.023 -0.263 -0.052
-1.891 -0.052 3.848
0.003 0.000 -0.001
0.000 0.000 0.000
0.002 0.000 0.000

atensor 6 H
-2.460 1.243 -1.027
1.243 1.387 -3.481
-1.027 -3.481 0.881
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
-0.199 0.224 -0.535
0.224 0.496 -1.815
-0.535 -1.815 3.842
0.000 0.001 0.000
0.001 0.003 -0.001
0.001 0.002 0.000

atensor 8 H
0.288 -2.136 2.995
-2.136 -1.363 -2.052
2.995 -2.052 0.880
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.300 -0.386 1.560
-0.386 0.002 -1.070
1.560 -1.070 3.845
0.002 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

```
atensor 10 H
0.049 2.214 2.877
2.214 -1.126 2.213
2.877 2.213 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.260 0.400 1.500
0.400 0.048 1.154
1.499 1.154 3.850
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.460 1.242 1.026
1.242 1.387 3.482
1.026 3.482 0.882
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
-0.199 0.224 0.534
0.224 0.496 1.815
0.534 1.815 3.842
0.000 0.001 0.000
0.001 0.003 0.001
-0.001 -0.002 0.000

atensor 14 H
0.287 -2.136 -2.994
-2.136 -1.367 2.051
-2.994 2.051 0.878
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.301 -0.386 -1.560
-0.386 0.002 1.069
-1.560 1.069 3.850
0.002 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.047 2.214 -2.876
2.214 -1.126 -2.213
-2.876 -2.213 0.877
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.261 0.400 -1.499
0.400 0.049 -1.154
-1.499 -1.154 3.853
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.001 0.000

atensor 18 H
-2.313 -1.446 1.215
```

-1.446 1.239 -3.420
1.215 -3.420 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.173 -0.261 0.633
-0.261 0.469 -1.783
0.633 -1.783 3.841
0.000 -0.001 0.000
-0.001 0.003 -0.001
-0.001 0.002 0.000

atensor 20 C
0.561 0.022 1.891
0.022 -0.265 0.051
1.891 0.051 3.842
0.003 0.000 0.001
0.000 0.000 0.000
-0.002 0.000 0.000

atensor 21 H
1.754 0.125 3.628
0.125 -2.819 0.099
3.628 0.099 0.885
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-1690.597 2.444 0.174
2.444 -1690.316 -0.122
0.174 -0.122 -21.027
1925.632 0.000 0.002
0.000 1925.631 -0.001
0.002 -0.001 1944.796

orbtensor 2 H
1.411 7.124 0.886
7.124 -16.026 -2.364
0.886 -2.364 1.217
24.448 -6.381 -0.896
-6.381 40.136 2.519
-0.896 2.519 23.017

orbtensor 3 C
-212.303 19.378 7.433
19.378 -259.844 -16.205
7.433 -16.205 -66.871
251.926 -0.359 -1.394
-0.359 252.820 3.912
-1.394 3.912 231.155

orbtensor 4 H
-18.679 -0.632 2.484
-0.632 3.866 0.024
2.484 0.024 1.215
42.388 0.553 -2.674
0.553 22.194 -0.073
-2.674 -0.073 23.014

orbtensor 5 C
-269.254 -2.965 18.559
-2.965 -205.819 -1.312
18.559 -1.312 -66.641
252.948 0.033 -4.154

0.033 251.804 -0.114
-4.154 -0.114 231.159

orbtensor 6 H
2.185 -6.043 0.682
-6.043 -16.677 2.330
0.682 2.330 1.208
23.798 5.487 -0.756
5.487 40.786 -2.565
-0.756 -2.565 23.016

orbtensor 7 C
-209.749 -15.483 3.286
-15.483 -260.896 17.229
3.286 17.229 -66.746
251.888 0.311 -1.178
0.311 252.853 -3.982
-1.178 -3.982 231.152

orbtensor 8 H
-11.491 10.551 -2.118
10.551 -3.320 1.438
-2.118 1.438 1.223
35.935 -9.432 2.206
-9.432 28.643 -1.512
2.206 -1.512 23.014

orbtensor 9 C
-249.185 29.638 -14.804
29.638 -225.738 10.933
-14.804 10.933 -66.786
252.574 -0.536 3.423
-0.536 252.160 -2.350
3.423 -2.350 231.154

orbtensor 10 H
-10.150 -10.855 -1.937
-10.855 -4.464 -1.427
-1.937 -1.427 1.207
34.885 9.774 2.120
9.774 29.696 1.631
2.120 1.631 23.015

orbtensor 11 C
-242.541 -30.007 -14.405
-30.007 -229.953 -10.655
-14.405 -10.655 -66.597
252.513 0.557 3.290
0.557 252.220 2.533
3.290 2.533 231.152

orbtensor 12 H
2.186 -6.041 -0.679
-6.041 -16.677 -2.334
-0.679 -2.334 1.208
23.796 5.484 0.756
5.484 40.787 2.566
0.756 2.566 23.017

orbtensor 13 C
-209.731 -15.472 -3.264
-15.472 -260.898 -17.228
-3.264 -17.228 -66.765
251.887 0.310 1.172
0.310 252.853 3.985
1.172 3.985 231.155

orbtensor 14 H
-11.495 10.549 2.122
10.549 -3.316 -1.443
2.122 -1.443 1.227
35.939 -9.431 -2.209
-9.431 28.640 1.513
-2.209 1.513 23.014

orbtensor 15 C
-249.199 29.640 14.821
29.640 -225.739 -10.954
14.821 -10.954 -66.797
252.575 -0.536 -3.428
-0.536 252.162 2.350
-3.428 2.350 231.155

orbtensor 16 H
-10.147 -10.857 1.935
-10.857 -4.466 1.430
1.935 1.430 1.216
34.881 9.775 -2.120
9.775 29.699 -1.631
-2.120 -1.631 23.014

orbtensor 17 C
-242.537 -30.012 14.407
-30.012 -229.975 10.620
14.407 10.620 -66.602
252.511 0.556 -3.294
0.556 252.222 -2.531
-3.294 -2.531 231.151

orbtensor 18 H
1.407 7.127 -0.883
7.127 -16.025 2.365
-0.883 2.365 1.216
24.450 -6.384 0.894
-6.384 40.135 -2.517
0.894 -2.517 23.016

orbtensor 19 C
-212.316 19.392 -7.410
19.392 -259.847 16.165
-7.410 16.165 -66.880
251.927 -0.362 1.388
-0.362 252.822 -3.910
1.388 -3.910 231.153

orbtensor 20 C
-269.237 -2.979 -18.507
-2.979 -205.804 1.301
-18.507 1.301 -66.648
252.947 0.032 4.151
0.032 251.802 0.116
4.151 0.116 231.159

orbtensor 21 H
-18.676 -0.636 -2.486
-0.636 3.868 -0.022
-2.486 -0.022 1.220
42.388 0.556 2.672
0.556 22.194 0.073
2.672 0.073 23.014

gtensor (ppt)
-0.152 0.000 0.000
0.000 -0.152 0.000

```

0.000    0.000   -0.161
-0.183   -0.008    0.000
-0.008   -0.183    0.000
0.000    0.000   -0.375

```

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-101.0260	798.03967	96063.03689	0.07797	96063.11485	96861.15452
2	H	-0.0657	24.73433	15.51019	0.00656	15.51675	40.25109
3	C	1.3817	65.62767	-1297.57504	0.07674	-1297.49831	-1231.87064
4	H	-0.0627	24.66600	14.80161	0.00755	14.80916	39.47516
5	C	1.3833	64.73233	-1299.14027	0.07752	-1299.06275	-1234.33042
6	H	-0.0640	24.77200	15.11653	0.00825	15.12479	39.89679
7	C	1.3807	66.16733	-1296.63591	0.07793	-1296.55798	-1230.39065
8	H	-0.0650	24.66800	15.35273	0.00613	15.35886	40.02686
9	C	1.3833	64.72633	-1299.14027	0.07640	-1299.06387	-1234.33754
10	H	-0.0660	24.72967	15.58893	0.00886	15.59779	40.32746
11	C	1.3870	65.59800	-1302.58378	0.07842	-1302.50536	-1236.90736
12	H	-0.0637	24.77233	15.03780	0.00826	15.04606	39.81839
13	C	1.3807	66.16700	-1296.63591	0.07793	-1296.55798	-1230.39098
14	H	-0.0673	24.66967	15.90385	0.00613	15.90998	40.57965
15	C	1.3853	64.71900	-1301.01855	0.07650	-1300.94205	-1236.22305
16	H	-0.0673	24.73233	15.90385	0.00886	15.91271	40.64505
17	C	1.3887	65.59000	-1304.14901	0.07846	-1304.07055	-1238.48055
18	H	-0.0650	24.73300	15.35273	0.00655	15.35928	40.09228
19	C	1.3800	65.61967	-1296.00982	0.07670	-1295.93312	-1230.31345
20	C	1.3803	64.73967	-1296.32286	0.07743	-1296.24543	-1231.50577
21	H	-0.0600	24.66933	14.17175	0.00755	14.17930	38.84863
C Average		1.3831	65.36870	-1298.92114	0.07740	-1298.84374	-1233.47504
H Average		-0.0647	24.71467	15.27400	0.00747	15.28147	39.99614

6MnCp2-STO-PBE0-TZ2P-DZ

Temperature: 390

Spin: 2.5

atensor 1 Mn

```

-105.581 -0.004 -0.002
-0.004 -105.576 -0.002
-0.002 -0.002 -101.040
-2.545 0.000 0.000
0.000 -2.544 0.000
0.000 0.000 -2.942

```

atensor 2 H

```

-2.416 -1.461 -1.230
-1.461 1.175 3.461
-1.230 3.461 0.662
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

```

atensor 3 C

```

-0.222 -0.278 -0.635
-0.278 0.459 1.779
-0.635 1.779 3.740
0.001 -0.001 -0.001
-0.001 0.004 0.002

```

0.001 -0.002 0.000

atensor 4 H
1.699 0.126 -3.671
0.126 -2.922 -0.100
-3.671 -0.100 0.673
0.001 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.567 0.024 -1.892
0.024 -0.311 -0.052
-1.892 -0.052 3.755
0.004 0.000 -0.002
0.000 0.001 0.000
0.002 0.000 0.000

atensor 6 H
-2.560 1.256 -1.040
1.256 1.328 -3.523
-1.040 -3.523 0.668
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 7 C
-0.249 0.239 -0.537
0.239 0.488 -1.811
-0.537 -1.811 3.739
0.001 0.001 0.000
0.001 0.004 -0.002
0.001 0.002 0.000

atensor 8 H
0.206 -2.160 3.029
-2.160 -1.462 -2.077
3.029 -2.077 0.655
0.000 0.000 0.001
0.000 0.000 -0.001
0.000 0.000 0.000

atensor 9 C
0.279 -0.410 1.561
-0.410 -0.040 -1.068
1.561 -1.068 3.742
0.003 -0.002 0.001
-0.002 0.002 -0.001
-0.002 0.001 0.000

atensor 10 H
-0.036 2.238 2.911
2.238 -1.223 2.239
2.911 2.239 0.654
0.000 0.000 0.001
0.000 0.000 0.001
0.000 0.000 0.000

atensor 11 C
0.233 0.425 1.500
0.425 0.007 1.153
1.500 1.153 3.745
0.003 0.002 0.001
0.002 0.002 0.001
-0.002 -0.001 0.000

atensor 12 H

-2.560 1.255 1.039
1.255 1.328 3.524
1.039 3.524 0.669
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

atensor 13 C
-0.250 0.239 0.537
0.239 0.487 1.811
0.537 1.811 3.739
0.001 0.001 0.000
0.001 0.004 0.002
-0.001 -0.002 0.000

atensor 14 H
0.204 -2.159 -3.029
-2.159 -1.466 2.075
-3.029 2.075 0.653
0.000 0.000 -0.001
0.000 0.000 0.001
0.000 0.000 0.000

atensor 15 C
0.279 -0.410 -1.561
-0.410 -0.040 1.067
-1.561 1.067 3.745
0.003 -0.002 -0.001
-0.002 0.002 0.001
0.002 -0.001 0.000

atensor 16 H
-0.039 2.239 -2.910
2.239 -1.224 -2.239
-2.910 -2.239 0.651
0.000 0.000 -0.001
0.000 0.000 -0.001
0.000 0.000 0.000

atensor 17 C
0.234 0.425 -1.500
0.425 0.008 -1.153
-1.500 -1.153 3.748
0.003 0.002 -0.001
0.002 0.002 -0.001
0.002 0.001 0.000

atensor 18 H
-2.414 -1.461 1.231
-1.461 1.176 -3.461
1.231 -3.461 0.663
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 19 C
-0.223 -0.278 0.635
-0.278 0.458 -1.780
0.635 -1.779 3.737
0.001 -0.001 0.001
-0.001 0.004 -0.002
-0.001 0.002 0.000

atensor 20 C
0.567 0.024 1.893
0.024 -0.312 0.052
1.893 0.052 3.750

0.004 0.000 0.002
0.000 0.001 0.000
-0.002 0.000 0.000

atensor 21 H
1.703 0.127 3.672
0.127 -2.919 0.101
3.672 0.101 0.677
0.001 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-1700.609 7.778 0.202
7.778 -1706.276 -0.041
0.202 -0.041 26.983
1934.334 -0.001 0.001
-0.001 1934.339 0.000
0.001 0.000 1940.435

orbtensor 2 H
1.344 5.448 0.614
5.448 -12.204 -1.846
0.614 -1.846 3.238
25.213 -5.575 -0.915
-5.575 38.930 2.572
-0.915 2.572 23.970

orbtensor 3 C
-184.888 12.434 6.550
12.434 -220.590 -19.460
6.550 -19.460 -58.477
261.226 7.081 -0.501
7.081 243.904 1.429
-0.501 1.429 242.389

orbtensor 4 H
-14.238 -0.484 2.002
-0.484 3.184 0.046
2.002 0.046 3.248
40.875 0.483 -2.728
0.483 23.238 -0.075
-2.728 -0.075 23.963

orbtensor 5 C
-227.376 -1.943 19.264
-1.943 -182.059 1.348
19.264 1.348 -58.284
241.308 -0.616 -1.493
-0.616 263.745 -0.038
-1.493 -0.038 242.374

orbtensor 6 H
1.835 -4.714 0.591
-4.714 -12.822 1.860
0.591 1.860 3.122
24.637 4.793 -0.773
4.793 39.491 -2.619
-0.773 -2.619 23.964

orbtensor 7 C
-184.810 -11.942 5.920
-11.942 -223.044 18.552
5.920 18.552 -56.289
261.927 -6.097 -0.420
-6.097 243.156 -1.452
-0.420 -1.452 242.368

orbtensor 8 H
-8.570 8.152 -1.532
8.152 -2.392 1.102
-1.532 1.102 3.029
35.250 -8.245 2.247
-8.245 28.875 -1.541
2.247 -1.541 23.961

orbtensor 9 C
-210.620 21.180 -17.071
21.180 -196.869 11.135
-17.071 11.135 -57.135
248.525 10.433 1.243
10.433 256.599 -0.850
1.243 -0.850 242.373

orbtensor 10 H
-7.762 -8.462 -1.533
-8.462 -3.369 -1.267
-1.533 -1.267 3.121
34.323 8.543 2.158
8.543 29.786 1.661
2.158 1.661 23.950

orbtensor 11 C
-210.185 -22.676 -14.805
-22.676 -200.749 -11.319
-14.805 -11.319 -56.416
249.686 -10.817 1.189
-10.817 255.435 0.915
1.189 0.915 242.354

orbtensor 12 H
1.838 -4.711 -0.592
-4.711 -12.823 -1.863
-0.592 -1.863 3.127
24.635 4.790 0.772
4.790 39.492 2.620
0.772 2.620 23.964

orbtensor 13 C
-184.802 -11.920 -5.886
-11.920 -223.055 -18.540
-5.886 -18.540 -56.404
261.924 -6.098 0.413
-6.098 243.155 1.453
0.413 1.453 242.369

orbtensor 14 H
-8.575 8.152 1.537
8.152 -2.390 -1.105
1.537 -1.105 3.031
35.254 -8.244 -2.249
-8.244 28.873 1.542
-2.249 1.542 23.961

orbtensor 15 C
-210.658 21.180 17.082
21.180 -196.891 -11.131
17.082 -11.131 -57.229
248.531 10.430 -1.244
10.430 256.609 0.849
-1.244 0.849 242.372

orbtensor 16 H
-7.760 -8.464 1.535

```

-8.464   -3.373   1.269
1.535    1.269    3.126
34.321   8.545    -2.158
8.545    29.789   -1.661
-2.158   -1.661    23.949

```

```

orbtensor 17 C
-210.212 -22.681  14.805
-22.681 -200.769  11.278
14.805  11.278 -56.528
249.695 -10.817 -1.193
-10.817 255.438 -0.910
-1.193  -0.910 242.353

```

```

orbtensor 18 H
1.344    5.450   -0.616
5.450   -12.200  1.848
-0.616   1.848   3.244
25.214   -5.577  0.914
-5.577   38.929 -2.570
0.914   -2.570  23.970

```

```

orbtensor 19 C
-184.886  12.425  -6.519
12.425 -220.576  19.409
-6.519  19.409 -58.616
261.217   7.087   0.496
7.087  243.902 -1.430
0.496  -1.430 242.384

```

```

orbtensor 20 C
-227.360  -1.940  -19.211
-1.940 -182.036  -1.366
-19.211  -1.366 -58.407
241.301  -0.621   1.493
-0.621  263.737   0.041
1.493   0.041 242.379

```

```

orbtensor 21 H
-14.235  -0.487  -2.004
-0.487   3.185  -0.047
-2.004  -0.047  3.254
40.874   0.485  2.727
0.485   23.238  0.075
2.727   0.075 23.964

```

```

gtensor (ppt)
-0.141   0.000   0.000
0.000  -0.141   0.000
0.000   0.000  -0.162
0.199  -0.022   0.000
-0.022   0.224   0.000
0.000   0.000  -0.381

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-106.7427	809.73533	101512.45668	0.26811	101512.72480	102322.46013
2	H	-0.1927	26.83033	45.51316	0.01633	45.52949	72.35982
3	C	1.3273	94.52133	-1246.71545	0.22820	-1246.48725	-1151.96591
4	H	-0.1830	26.75667	43.22963	0.02314	43.25277	70.00944

5	C	1.3387	93.23600	-1257.36043	0.23370	-1257.12673	-1163.89073
6	H	-0.1877	26.74233	44.33202	0.02091	44.35293	71.09526
7	C	1.3277	94.43600	-1247.02854	0.23154	-1246.79700	-1152.36100
8	H	-0.2003	26.71767	47.32424	0.01772	47.34196	74.05962
9	C	1.3287	94.29100	-1247.96780	0.22931	-1247.73849	-1153.44749
10	H	-0.2017	26.68300	47.63921	0.02510	47.66431	74.34731
11	C	1.3300	93.37500	-1249.22015	0.23506	-1248.98509	-1155.61009
12	H	-0.1873	26.74433	44.25328	0.02092	44.27420	71.01854
13	C	1.3270	94.39567	-1246.40236	0.23160	-1246.17076	-1151.77509
14	H	-0.2030	26.71800	47.95418	0.01774	47.97192	74.68992
15	C	1.3297	94.24467	-1248.90706	0.22951	-1248.67756	-1154.43289
16	H	-0.2040	26.68400	48.19041	0.02509	48.21549	74.89949
17	C	1.3317	93.32567	-1250.78559	0.23519	-1250.55040	-1157.22473
18	H	-0.1913	26.83367	45.19819	0.01632	45.21451	72.04818
19	C	1.3257	94.47500	-1245.15001	0.22807	-1244.92194	-1150.44694
20	C	1.3367	93.20467	-1255.48191	0.23341	-1255.24849	-1162.04383
21	H	-0.1793	26.76000	42.36346	0.02315	42.38662	69.14662
C Average		1.3303	93.95050	-1249.50193	0.23156	-1249.27037	-1155.31987
H Average		-0.1930	26.74700	45.59978	0.02064	45.62042	72.36742

=====

6MnCp2-STO-PBE0-TZ2P-TZ2P

Temperature: 390

Spin: 2.5

atensor 1 Mn

-100.654 -0.001 -0.002
-0.001 -100.671 -0.001
-0.002 -0.001 -96.303
-2.666 0.000 0.000
0.000 -2.666 0.000
0.000 0.000 -2.988

atensor 2 H

-2.342 -1.449 -1.218
-1.449 1.219 3.426
-1.218 3.426 0.876
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C

-0.019 -0.262 -0.631
-0.262 0.626 1.776
-0.631 1.776 3.960
0.000 -0.001 0.000
-0.001 0.003 0.001
0.001 -0.002 0.000

atensor 4 H

1.732 0.125 -3.634
0.125 -2.851 -0.099
-3.634 -0.099 0.878
0.000 0.000 0.000
0.000 0.001 0.000
0.000 0.000 0.000

atensor 5 C

0.719 0.023 -1.884
0.023 -0.111 -0.051
-1.884 -0.051 3.965
0.004 0.000 -0.001
0.000 0.000 0.000
0.002 0.000 0.000

atensor 6 H
-2.488 1.245 -1.029
1.245 1.367 -3.488
-1.029 -3.488 0.877
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 7 C
-0.046 0.225 -0.533
0.225 0.653 -1.808
-0.533 -1.808 3.959
0.000 0.001 0.000
0.001 0.003 -0.001
0.001 0.002 0.000

atensor 8 H
0.269 -2.141 3.000
-2.141 -1.386 -2.056
3.000 -2.056 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.452 -0.388 1.554
-0.388 0.153 -1.066
1.554 -1.066 3.958
0.003 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.029 2.219 2.882
2.219 -1.148 2.217
2.882 2.217 0.878
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.411 0.402 1.494
0.402 0.199 1.150
1.494 1.150 3.962
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.488 1.245 1.028
1.245 1.368 3.488
1.028 3.488 0.879
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 13 C
-0.046 0.225 0.533
0.225 0.653 1.808
0.533 1.808 3.959
0.000 0.001 0.000
0.001 0.003 0.001
-0.001 -0.002 0.000

atensor 14 H
0.267 -2.140 -3.000
-2.140 -1.390 2.055

-3.000 2.055 0.877
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.452 -0.387 -1.554
-0.387 0.152 1.065
-1.554 1.065 3.961
0.002 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.027 2.219 -2.881
2.219 -1.149 -2.217
-2.881 -2.217 0.875
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.413 0.402 -1.493
0.402 0.200 -1.150
-1.493 -1.150 3.966
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.001 0.000

atensor 18 H
-2.341 -1.449 1.218
-1.449 1.220 -3.426
1.218 -3.426 0.875
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.020 -0.262 0.631
-0.262 0.626 -1.776
0.631 -1.776 3.958
0.000 -0.001 0.000
-0.001 0.003 -0.001
-0.001 0.002 0.000

atensor 20 C
0.718 0.022 1.884
0.022 -0.112 0.051
1.884 0.051 3.960
0.004 0.000 0.001
0.000 0.000 0.000
-0.002 0.000 0.000

atensor 21 H
1.735 0.126 3.635
0.126 -2.848 0.099
3.635 0.099 0.881
0.000 0.000 0.000
0.000 0.001 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-1691.589 2.358 0.229
2.358 -1693.124 -0.124
0.229 -0.124 -39.029
1937.094 0.001 0.001
0.001 1937.092 0.000

```

0.001      0.000 1940.007

orbtensor 2 H
-1.443      5.334      1.144
5.334     -14.907     -3.240
1.144      -3.240     -0.222
27.382     -4.788     -1.141
-4.788     39.154      3.209
-1.141      3.209     25.096

orbtensor 3 C
-205.475     13.564      6.170
13.564    -244.395    -16.946
6.170     -16.946    -65.735
251.918      2.726     -1.780
2.726     245.226      5.007
-1.780      5.007     232.266

orbtensor 4 H
-16.982     -0.331      3.530
-0.331      0.172      0.102
3.530      0.102     -0.152
40.844      0.415     -3.405
0.415     25.690     -0.093
-3.405     -0.093     25.093

orbtensor 5 C
-251.819     -0.976     18.185
-0.976    -199.127      0.823
18.185      0.823    -65.947
244.268     -0.236     -5.312
-0.236     252.893     -0.144
-5.312     -0.144     232.271

orbtensor 6 H
-1.157     -4.673      1.010
-4.673    -15.554      3.379
1.010      3.379     -0.126
26.894      4.117     -0.964
4.117     39.641     -3.267
-0.964     -3.267     25.095

orbtensor 7 C
-205.274    -15.490      5.899
-15.490   -246.497     17.104
5.899     17.104    -65.756
252.196     -2.344     -1.506
-2.344    244.945     -5.096
-1.506     -5.096     232.267

orbtensor 8 H
-11.374      8.012     -2.896
8.012     -5.102      1.953
-2.896      1.953     -0.172
36.001     -7.078      2.810
-7.078     30.528     -1.926
2.810     -1.926     25.093

orbtensor 9 C
-235.289     22.472    -14.901
22.472   -214.865     10.137
-14.901     10.137    -65.771
247.009      4.028      4.384
4.028     250.122     -3.004
4.384     -3.004     232.269

orbtensor 10 H

```

-10.619	-8.269	-2.761
-8.269	-6.180	-2.106
-2.761	-2.106	-0.203
35.212	7.334	2.700
7.334	31.318	2.077
2.700	2.077	25.094

orbtensor 11 C

-232.877	-24.863	-15.016
-24.863	-217.919	-10.605
-15.016	-10.605	-66.026
247.460	-4.173	4.212
-4.173	249.677	3.241
4.212	3.241	232.268

orbtensor 12 H

-1.147	-4.672	-1.014
-4.672	-15.554	-3.379
-1.014	-3.379	-0.130
26.892	4.115	0.963
4.115	39.641	3.269
0.963	3.269	25.096

orbtensor 13 C

-205.264	-15.469	-5.873
-15.469	-246.501	-17.125
-5.873	-17.125	-65.747
252.195	-2.344	1.497
-2.344	244.943	5.100
1.497	5.100	232.270

orbtensor 14 H

-11.379	8.013	2.897
8.013	-5.104	-1.951
2.897	-1.951	-0.173
36.004	-7.076	-2.812
-7.076	30.527	1.926
-2.812	1.926	25.093

orbtensor 15 C

-235.352	22.480	14.927
22.480	-214.895	-10.154
14.927	-10.154	-65.771
247.014	4.028	-4.387
4.028	250.129	3.004
-4.387	3.004	232.268

orbtensor 16 H

-10.615	-8.272	2.764
-8.272	-6.183	2.107
2.764	2.107	-0.212
35.211	7.335	-2.700
7.335	31.321	-2.077
-2.700	-2.077	25.093

orbtensor 17 C

-232.905	-24.861	15.043
-24.861	-217.938	10.589
15.043	10.589	-66.020
247.466	-4.174	-4.216
-4.174	249.679	-3.237
-4.216	-3.237	232.266

orbtensor 18 H

-1.441	5.336	-1.141
5.336	-14.907	3.235
-1.141	3.235	-0.222


```

27.384   -4.790    1.140
-4.790   39.154   -3.208
1.140    -3.208   25.096

```

```

orbtensor 19 C
-205.466  13.573  -6.146
13.573  -244.393  16.917
-6.146   16.917  -65.713
251.914   2.728   1.775
2.728  245.227  -5.007
1.775   -5.007  232.263

```

```

orbtensor 20 C
-251.812  -0.966  -18.166
-0.966 -199.103  -0.838
-18.166  -0.838  -65.940
244.260  -0.239   5.310
-0.239  252.884   0.148
5.310    0.148  232.272

```

```

orbtensor 21 H
-16.983  -0.333  -3.530
-0.333   0.172  -0.104
-3.530  -0.104  -0.158
40.843   0.417   3.404
0.417   25.690   0.094
3.404    0.094  25.093

```

```

gtensor (ppt)
-0.143   0.000   0.000
0.000  -0.143   0.000
0.000   0.000  -0.160
-0.121   0.001   0.000
0.001  -0.131   0.000
0.000   0.000  -0.271

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-101.9827	796.81700	96976.53348	0.06903	96976.60251	97773.41951
2	H	-0.0823	25.02000	19.44756	0.00692	19.45448	44.47448
3	C	1.5233	71.26833	-1430.67599	0.06232	-1430.61367	-1359.34534
4	H	-0.0800	24.88833	18.89641	0.00519	18.90161	43.78994
5	C	1.5257	70.84633	-1432.86739	0.06113	-1432.80626	-1361.95992
6	H	-0.0813	24.93100	19.21135	0.00677	19.21812	44.14912
7	C	1.5230	70.62700	-1430.36293	0.06219	-1430.30074	-1359.67374
8	H	-0.0793	24.99133	18.73894	0.00595	18.74489	43.73623
9	C	1.5223	71.15833	-1429.73681	0.06159	-1429.67522	-1358.51689
10	H	-0.0803	24.87400	18.97515	0.00570	18.98085	43.85485
11	C	1.5250	70.86100	-1432.24128	0.06144	-1432.17983	-1361.31883
12	H	-0.0803	24.93267	18.97515	0.00677	18.98192	43.91459
13	C	1.5230	70.63200	-1430.36293	0.06219	-1430.30074	-1359.66874
14	H	-0.0820	24.98933	19.36882	0.00595	19.37478	44.36411
15	C	1.5227	71.13100	-1430.04987	0.06166	-1429.98821	-1358.85721
16	H	-0.0823	24.87167	19.44756	0.00569	19.45325	44.32492
17	C	1.5273	70.84933	-1434.43268	0.06148	-1434.37120	-1363.52187
18	H	-0.0820	25.02133	19.36882	0.00691	19.37574	44.39707
19	C	1.5223	71.27733	-1429.73681	0.06229	-1429.67452	-1358.39719
20	C	1.5233	70.85367	-1430.67599	0.06107	-1430.61492	-1359.76125
21	H	-0.0770	24.88567	18.18780	0.00519	18.19299	43.07866

C Average	1.5238	70.95043	-1431.11427	0.06174	-1431.05253	-1360.10210
H Average	-0.0807	24.94053	19.06176	0.00610	19.06786	44.00840

=====
6MnCp2-STO-PBE0-TZ2P-QZ4P
Temperature: 390
Spin: 2.5

atensor 1 Mn
-99.426 -0.002 -0.002
-0.002 -99.442 -0.001
-0.002 -0.001 -95.068
-2.704 0.000 0.000
0.000 -2.704 0.000
0.000 0.000 -3.002

atensor 2 H
-2.304 -1.442 -1.217
-1.442 1.241 3.424
-1.217 3.424 0.888
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 3 C
-0.166 -0.261 -0.633
-0.261 0.476 1.781
-0.633 1.781 3.823
0.000 -0.001 0.000
-0.001 0.003 0.001
0.001 -0.002 0.000

atensor 4 H
1.751 0.125 -3.632
0.125 -2.812 -0.099
-3.632 -0.099 0.890
0.000 0.000 0.000
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C
0.569 0.022 -1.889
0.022 -0.256 -0.051
-1.889 -0.051 3.829
0.003 0.000 -0.001
0.000 -0.001 0.000
0.002 0.000 0.000

atensor 6 H
-2.450 1.240 -1.028
1.240 1.388 -3.485
-1.028 -3.485 0.890
0.001 0.000 0.000
0.000 0.000 0.000
0.000 0.001 0.000

atensor 7 C
-0.192 0.224 -0.535
0.224 0.503 -1.813
-0.535 -1.813 3.822
0.000 0.001 0.000
0.001 0.003 -0.001
0.001 0.002 0.000

atensor 8 H
0.294 -2.131 2.998

-2.131 -1.354 -2.055
2.998 -2.055 0.891
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.304 -0.386 1.558
-0.386 0.006 -1.069
1.558 -1.069 3.820
0.002 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.055 2.209 2.881
2.209 -1.117 2.216
2.881 2.216 0.889
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.263 0.400 1.498
0.400 0.051 1.153
1.498 1.153 3.826
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.450 1.239 1.027
1.239 1.389 3.486
1.027 3.486 0.891
0.001 0.000 0.000
0.000 0.000 0.000
0.000 -0.001 0.000

atensor 13 C
-0.192 0.224 0.534
0.224 0.503 1.813
0.534 1.813 3.822
0.000 0.001 0.000
0.001 0.003 0.001
-0.001 -0.002 0.000

atensor 14 H
0.292 -2.131 -2.998
-2.131 -1.357 2.053
-2.998 2.053 0.889
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.304 -0.385 -1.559
-0.385 0.006 1.068
-1.559 1.068 3.825
0.002 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.053 2.209 -2.879
2.209 -1.117 -2.216
-2.879 -2.216 0.887
0.000 0.000 0.000

0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.264 0.400 -1.497
0.400 0.053 -1.153
-1.497 -1.153 3.829
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.001 0.000

atensor 18 H
-2.303 -1.443 1.217
-1.443 1.242 -3.424
1.217 -3.424 0.888
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.167 -0.261 0.633
-0.261 0.475 -1.781
0.633 -1.781 3.820
0.000 -0.001 0.000
-0.001 0.003 -0.001
-0.001 0.002 0.000

atensor 20 C
0.568 0.022 1.889
0.022 -0.258 0.051
1.889 0.051 3.823
0.003 0.000 0.001
0.000 -0.001 0.000
-0.002 0.000 0.000

atensor 21 H
1.754 0.125 3.633
0.125 -2.809 0.099
3.633 0.099 0.893
0.000 0.000 0.000
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1680.155 16.903 0.162
16.903 -1687.099 -0.104
0.162 -0.104 -132.410
1925.433 0.001 0.002
0.001 1925.430 -0.001
0.002 -0.001 1944.437

orbtensor 2 H
1.302 7.083 0.972
7.083 -16.125 -2.600
0.972 -2.600 1.160
24.465 -6.371 -0.864
-6.371 40.125 2.430
-0.864 2.430 23.028

orbtensor 3 C
-213.054 18.412 5.548
18.412 -260.323 -15.190
5.548 -15.190 -66.156
252.165 -0.316 -1.305
-0.316 252.949 3.664
-1.305 3.664 231.109

orbtensor 4 H
-18.655 -0.569 2.709
-0.569 3.731 0.052
2.709 0.052 1.157
42.375 0.552 -2.579
0.552 22.216 -0.071
-2.579 -0.071 23.026

orbtensor 5 C
-267.749 -1.312 16.058
-1.312 -205.389 -1.392
16.058 -1.392 -66.139
253.068 0.029 -3.891
0.029 252.060 -0.106
-3.891 -0.106 231.113

orbtensor 6 H
2.100 -6.011 0.651
-6.011 -16.771 2.591
0.651 2.591 1.161
23.818 5.478 -0.730
5.478 40.775 -2.474
-0.730 -2.474 23.028

orbtensor 7 C
-210.387 -14.764 3.342
-14.764 -261.165 15.402
3.342 15.402 -66.121
252.134 0.274 -1.103
0.274 252.981 -3.730
-1.103 -3.730 231.107

orbtensor 8 H
-11.471 10.513 -2.289
10.513 -3.505 1.614
-2.289 1.614 1.154
35.933 -9.415 2.127
-9.415 28.653 -1.459
2.127 -1.459 23.026

orbtensor 9 C
-246.796 29.628 -12.492
29.628 -227.599 10.663
-12.492 10.663 -66.169
252.736 -0.470 3.206
-0.470 252.372 -2.201
3.206 -2.201 231.111

orbtensor 10 H
-10.186 -10.815 -2.038
-10.815 -4.542 -1.655
-2.038 -1.655 1.152
34.884 9.757 2.044
9.757 29.704 1.573
2.044 1.573 23.027

orbtensor 11 C
-241.997 -29.496 -12.401
-29.496 -229.477 -9.483
-12.401 -9.483 -66.128
252.682 0.489 3.082
0.489 252.423 2.373
3.082 2.373 231.110

orbtensor 12 H
2.114 -6.008 -0.670
-6.008 -16.767 -2.613

-0.670	-2.613	1.159
23.816	5.475	0.729
5.475	40.776	2.476
0.729	2.476	23.028

orbtensor 13 C

-210.346	-14.744	-3.351
-14.744	-261.153	-15.440
-3.351	-15.440	-66.138
252.133	0.273	1.096
0.273	252.980	3.733
1.096	3.733	231.109

orbtensor 14 H

-11.460	10.510	2.330
10.510	-3.499	-1.614
2.330	-1.614	1.149
35.937	-9.414	-2.130
-9.414	28.651	1.460
-2.130	1.460	23.026

orbtensor 15 C

-246.784	29.625	12.589
29.625	-227.589	-10.693
12.589	-10.693	-66.169
252.738	-0.470	-3.211
-0.470	252.374	2.201
-3.211	2.201	231.111

orbtensor 16 H

-10.168	-10.814	2.077
-10.814	-4.543	1.658
2.077	1.658	1.165
34.880	9.758	-2.045
9.758	29.708	-1.573
-2.045	-1.573	23.026

orbtensor 17 C

-241.954	-29.502	12.477
-29.502	-229.495	9.479
12.477	9.479	-66.104
252.680	0.488	-3.086
0.488	252.426	-2.371
-3.086	-2.371	231.108

orbtensor 18 H

1.311	7.086	-0.996
7.086	-16.119	2.616
-0.996	2.616	1.151
24.467	-6.373	0.863
-6.373	40.124	-2.428
0.863	-2.428	23.027

orbtensor 19 C

-213.024	18.424	-5.558
18.424	-260.311	15.187
-5.558	15.187	-66.155
252.166	-0.318	1.300
-0.318	252.951	-3.662
1.300	-3.662	231.108

orbtensor 20 C

-267.699	-1.320	-16.091
-1.320	-205.371	1.378
-16.091	1.378	-66.144
253.066	0.028	3.887
0.028	252.058	0.109

3.887 0.109 231.113

orbtensor 21 H

-18.637 -0.572 -2.740
-0.572 3.737 -0.053
-2.740 -0.053 1.163
42.375 0.555 2.577
0.555 22.216 0.071
2.577 0.071 23.026

gtensor (ppt)

-0.150 0.000 0.000
0.000 -0.150 0.000
0.000 0.000 -0.161
-0.293 -0.053 0.000
-0.053 -0.267 0.000
0.000 0.000 -0.053

averaging

C Average:3,5,7,9,11,13,15,17,19,20

H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.

Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-100.7820	765.21200	95833.12980	-0.09275	95833.03705	96598.24905
2	H	-0.0583	24.65167	13.77839	-0.01586	13.76253	38.41420
3	C	1.3787	65.56333	-1294.78609	-0.08822	-1294.87430	-1229.31097
4	H	-0.0567	24.61667	13.38473	-0.00519	13.37954	37.99620
5	C	1.3813	65.65467	-1297.29051	-0.08062	-1297.37113	-1231.71647
6	H	-0.0570	24.70367	13.46346	-0.00484	13.45862	38.16229
7	C	1.3787	66.18300	-1294.78609	-0.08022	-1294.86631	-1228.68331
8	H	-0.0563	24.59667	13.30599	-0.01609	13.28990	37.88657
9	C	1.3777	65.21833	-1293.84693	-0.08832	-1293.93525	-1228.71691
10	H	-0.0577	24.67967	13.62093	0.00177	13.62269	38.30236
11	C	1.3810	66.20433	-1296.97746	-0.07549	-1297.05295	-1230.84861
12	H	-0.0563	24.70867	13.30599	-0.00484	13.30115	38.00981
13	C	1.3787	66.19500	-1294.78609	-0.08022	-1294.86631	-1228.67131
14	H	-0.0587	24.60133	13.85713	-0.01609	13.84104	38.44237
15	C	1.3793	65.22700	-1295.41219	-0.08841	-1295.50061	-1230.27361
16	H	-0.0590	24.68933	13.93586	0.00177	13.93763	38.62697
17	C	1.3830	66.22033	-1298.85577	-0.07552	-1298.93130	-1232.71096
18	H	-0.0577	24.65367	13.62093	-0.01586	13.60507	38.25873
19	C	1.3770	65.57833	-1293.22083	-0.08817	-1293.30900	-1227.73066
20	C	1.3783	65.67433	-1294.47304	-0.08052	-1294.55356	-1228.87922
21	H	-0.0537	24.62667	12.67612	-0.00519	12.67093	37.29760
	C Average	1.3794	65.77187	-1295.44350	-0.08257	-1295.52607	-1229.75420
	H Average	-0.0571	24.65280	13.49495	-0.00804	13.48691	38.13971

6MnCp2-STO-PBE0-QZ4P-DZ

Temperature: 390

Spin: 2.5

atensor 1 Mn

-132.031 -0.002 -0.002
-0.002 -132.010 0.000
-0.002 0.000 -127.093
-4.008 0.000 0.000
0.000 -4.008 0.000
0.000 0.000 -4.381

atensor 2 H

-2.375 -1.460 -1.228
-1.460 1.214 3.453
-1.228 3.453 0.712
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

atensor 3 C
-0.193 -0.276 -0.632
-0.276 0.484 1.770
-0.632 1.770 3.717
0.001 -0.001 0.000
-0.001 0.004 0.001
0.001 -0.002 0.000

atensor 4 H
1.738 0.126 -3.663
0.126 -2.881 -0.100
-3.663 -0.100 0.724
0.001 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 5 C
0.591 0.024 -1.884
0.024 -0.283 -0.052
-1.884 -0.052 3.729
0.005 0.000 -0.001
0.000 0.001 0.000
0.002 0.000 0.000

atensor 6 H
-2.519 1.255 -1.037
1.255 1.367 -3.515
-1.037 -3.515 0.719
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 7 C
-0.221 0.238 -0.535
0.238 0.512 -1.803
-0.535 -1.803 3.715
0.001 0.001 0.000
0.001 0.004 -0.001
0.001 0.002 0.000

atensor 8 H
0.246 -2.159 3.022
-2.159 -1.422 -2.072
3.022 -2.072 0.706
0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.305 -0.408 1.553
-0.408 -0.012 -1.063
1.553 -1.063 3.719
0.003 -0.002 0.001
-0.002 0.002 -0.001
-0.002 0.001 0.000

atensor 10 H
0.005 2.237 2.904
2.237 -1.182 2.234
2.904 2.234 0.705

0.000 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.261 0.422 1.493
0.422 0.036 1.147
1.493 1.147 3.724
0.003 0.002 0.001
0.002 0.002 0.001
-0.002 -0.001 0.000

atensor 12 H
-2.519 1.254 1.037
1.254 1.367 3.516
1.037 3.516 0.720
0.000 0.000 0.000
0.000 0.001 0.001
0.000 0.000 0.000

atensor 13 C
-0.221 0.238 0.535
0.238 0.512 1.803
0.535 1.803 3.715
0.001 0.001 0.000
0.001 0.004 0.001
-0.001 -0.002 0.000

atensor 14 H
0.244 -2.158 -3.022
-2.158 -1.426 2.070
-3.022 2.070 0.703
0.000 0.000 -0.001
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.306 -0.407 -1.553
-0.407 -0.011 1.062
-1.553 1.062 3.723
0.003 -0.002 -0.001
-0.002 0.002 0.001
0.002 -0.001 0.000

atensor 16 H
0.001 2.238 -2.903
2.238 -1.183 -2.234
-2.903 -2.234 0.701
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.261 0.423 -1.493
0.423 0.037 -1.147
-1.493 -1.147 3.727
0.003 0.002 -0.001
0.002 0.002 -0.001
0.002 0.001 0.000

atensor 18 H
-2.374 -1.461 1.228
-1.461 1.215 -3.453
1.228 -3.453 0.713
0.000 0.000 0.000
0.000 0.001 -0.001
0.000 0.000 0.000

atensor 19 C
-0.194 -0.276 0.632
-0.276 0.484 -1.771
0.632 -1.771 3.714
0.001 -0.001 0.000
-0.001 0.004 -0.001
-0.001 0.002 0.000

atensor 20 C
0.591 0.024 1.884
0.024 -0.283 0.052
1.884 0.052 3.725
0.005 0.000 0.001
0.000 0.001 0.000
-0.002 0.000 0.000

atensor 21 H
1.742 0.127 3.664
0.127 -2.878 0.100
3.664 0.100 0.727
0.001 0.000 0.001
0.000 0.000 0.000
0.000 0.000 0.000

orbtensor 1 Mn
-1771.725 -3.997 -1.175
-3.997 -1763.060 0.466
-1.175 0.466 10.495
1933.579 -0.001 0.002
-0.001 1933.586 0.000
0.002 0.000 1943.407

orbtensor 2 H
2.193 4.403 0.501
4.403 -8.778 -1.111
0.501 -1.111 2.891
24.243 -4.437 -0.660
-4.437 35.153 1.860
-0.660 1.860 24.265

orbtensor 3 C
-175.565 12.304 3.775
12.304 -213.475 -14.953
3.775 -14.953 -60.534
246.296 7.098 -1.643
7.098 228.945 4.649
-1.643 4.649 239.593

orbtensor 4 H
-10.230 -0.404 1.376
-0.404 3.862 0.114
1.376 0.114 3.000
36.686 0.384 -1.981
0.384 22.652 -0.054
-1.981 -0.054 24.251

orbtensor 5 C
-215.888 -2.423 17.157
-2.423 -174.994 0.043
17.157 0.043 -60.857
226.306 -0.622 -4.913
-0.622 248.799 -0.129
-4.913 -0.129 239.599

orbtensor 6 H
2.786 -3.805 0.357

-3.805	-9.230	1.149
0.357	1.149	2.866
23.781	3.814	-0.558
3.814	35.597	-1.896
-0.558	-1.896	24.257

orbtensor 7 C

-176.969	-10.972	4.060
-10.972	-213.337	15.142
4.060	15.142	-59.815
246.997	-6.115	-1.382
-6.115	228.196	-4.731
-1.382	-4.731	239.578

orbtensor 8 H

-6.078	6.707	-0.971
6.707	-0.800	0.626
-0.971	0.626	2.661
32.226	-6.555	1.621
-6.555	27.160	-1.112
1.621	-1.112	24.257

orbtensor 9 C

-206.891	23.726	-13.557
23.726	-186.873	10.722
-13.557	10.722	-59.354
233.573	10.461	4.049
10.461	241.678	-2.776
4.049	-2.776	239.582

orbtensor 10 H

-5.214	-6.924	-0.907
-6.924	-1.320	-0.808
-0.907	-0.808	2.684
31.486	6.793	1.557
6.793	27.881	1.198
1.557	1.198	24.246

orbtensor 11 C

-203.855	-20.423	-13.738
-20.423	-190.386	-10.220
-13.738	-10.220	-58.401
234.734	-10.849	3.886
-10.849	240.510	2.993
3.886	2.993	239.563

orbtensor 12 H

2.555	-3.847	-0.281
-3.847	-8.881	-1.257
-0.281	-1.257	2.871
23.779	3.812	0.558
3.812	35.598	1.897
0.558	1.897	24.257

orbtensor 13 C

-173.073	-12.289	-8.545
-12.289	-210.893	-16.716
-8.545	-16.716	-60.468
246.996	-6.114	1.376
-6.114	228.195	4.730
1.376	4.730	239.580

orbtensor 14 H

-5.465	6.399	0.910
6.399	-0.586	-0.676
0.910	-0.676	2.665
32.229	-6.555	-1.624

-6.555	27.158	1.113
-1.624	1.113	24.257

orbtensor 15 C

-198.391	17.949	15.081
17.949	-185.557	-7.279
15.081	-7.279	-59.328
233.574	10.459	-4.051
10.459	241.682	2.774
-4.051	2.774	239.582

orbtensor 16 H

-4.901	-6.662	0.853
-6.662	-1.423	0.807
0.853	0.807	2.688
31.483	6.794	-1.558
6.794	27.883	-1.199
-1.558	-1.199	24.244

orbtensor 17 C

-198.467	-21.150	14.999
-21.150	-187.892	8.421
14.999	8.421	-58.348
234.737	-10.849	-3.889
-10.849	240.508	-2.990
-3.889	-2.990	239.564

orbtensor 18 H

2.206	4.400	-0.517
4.400	-8.531	1.186
-0.517	1.186	2.902
24.243	-4.438	0.660
-4.438	35.151	-1.859
0.660	-1.859	24.264

orbtensor 19 C

-175.893	15.716	-6.475
15.716	-208.193	17.367
-6.475	17.367	-61.267
246.286	7.103	1.640
7.103	228.942	-4.651
1.640	-4.651	239.589

orbtensor 20 C

-215.063	0.921	-16.579
0.921	-171.194	-1.163
-16.579	-1.163	-60.336
226.305	-0.626	4.914
-0.626	248.795	0.131
4.914	0.131	239.602

orbtensor 21 H

-10.093	-0.337	-1.223
-0.337	3.880	-0.066
-1.223	-0.066	3.007
36.685	0.386	1.980
0.386	22.652	0.054
1.980	0.054	24.252

gtensor (ppt)

-0.133	0.000	0.000
0.000	-0.133	0.000
0.000	0.000	-0.164
0.067	0.009	0.005
0.009	0.035	-0.002
0.005	-0.002	-0.346

averaging
 C Average:3,5,7,9,11,13,15,17,19,20
 H Average:2,4,6,8,10,12,14,16,18,21

Final results. Shifts and Shieldings in ppm.
 Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-134.5103	762.09400	127913.76200	0.20582	127913.96781	128676.06181
2	H	-0.1493	26.65567	35.27504	0.01882	35.29386	61.94952
3	C	1.3377	88.42000	-1256.36427	0.16382	-1256.20045	-1167.78045
4	H	-0.1393	26.74033	32.91287	0.01296	32.92583	59.66617
5	C	1.3477	87.65500	-1265.75648	0.16003	-1265.59646	-1177.94146
6	H	-0.1440	26.68567	34.01522	0.01594	34.03116	60.71682
7	C	1.3370	88.21667	-1255.73813	0.16003	-1255.57810	-1167.36143
8	H	-0.1567	26.47533	37.00730	0.01348	37.02078	63.49611
9	C	1.3390	87.23833	-1257.61657	0.15655	-1257.46001	-1170.22168
10	H	-0.1573	26.58767	37.16477	0.01139	37.17617	63.76383
11	C	1.3420	87.38833	-1260.43423	0.15605	-1260.27818	-1172.88985
12	H	-0.1437	26.72633	33.93648	0.01624	33.95272	60.67905
13	C	1.3370	90.11233	-1255.73813	0.16061	-1255.57751	-1165.46518
14	H	-0.1597	26.75267	37.71595	0.01651	37.73246	64.48512
15	C	1.3410	90.52067	-1259.49501	0.16287	-1259.33214	-1168.81147
16	H	-0.1603	26.65800	37.87342	0.01296	37.88638	64.54438
17	C	1.3433	90.03400	-1261.68652	0.15939	-1261.52713	-1171.49313
18	H	-0.1483	26.74500	35.03882	0.01677	35.05559	61.80059
19	C	1.3363	89.82133	-1255.11198	0.15952	-1254.95246	-1165.13113
20	C	1.3463	89.36967	-1264.50419	0.15402	-1264.35016	-1174.98050
21	H	-0.1360	26.79433	32.12548	0.01010	32.13559	58.92992
C Average		1.3407	88.87763	-1259.24455	0.15929	-1259.08526	-1170.20763
H Average		-0.1495	26.68210	35.30653	0.01452	35.32105	62.00315

6MnCp2-STO-PBE0-QZ4P-TZ2P
 Temperature: 390
 Spin: 2.5

atensor 1 Mn
 -130.015 0.001 -0.002
 0.001 -130.017 0.001
 -0.002 0.001 -125.374
 -4.088 0.000 0.000
 0.000 -4.088 0.000
 0.000 0.000 -4.410

atensor 2 H
 -2.362 -1.449 -1.217
 -1.449 1.200 3.425
 -1.217 3.425 0.851
 0.000 0.000 0.000
 0.000 0.000 0.000
 0.000 0.000 0.000

atensor 3 C
 -0.015 -0.263 -0.631
 -0.263 0.630 1.773
 -0.631 1.773 3.961
 0.000 -0.001 0.000
 -0.001 0.004 0.001
 0.001 -0.002 0.000

atensor 4 H
 1.714 0.125 -3.633
 0.125 -2.870 -0.099

-3.633 -0.099 0.855
0.000 0.000 0.000
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C
0.723 0.023 -1.881
0.023 -0.107 -0.051
-1.881 -0.051 3.965
0.004 0.000 -0.001
0.000 0.000 0.000
0.002 0.000 0.000

atensor 6 H
-2.508 1.246 -1.028
1.246 1.349 -3.487
-1.028 -3.487 0.853
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.001 0.000

atensor 7 C
-0.042 0.226 -0.533
0.226 0.657 -1.805
-0.533 -1.805 3.959
0.000 0.001 0.000
0.001 0.004 -0.001
0.001 0.002 0.000

atensor 8 H
0.250 -2.142 2.999
-2.142 -1.406 -2.056
2.999 -2.056 0.854
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.456 -0.388 1.552
-0.388 0.157 -1.064
1.552 -1.064 3.958
0.003 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.011 2.219 2.882
2.219 -1.167 2.216
2.882 2.216 0.854
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.416 0.402 1.492
0.402 0.203 1.148
1.492 1.148 3.963
0.003 0.002 0.001
0.002 0.001 0.001
-0.002 -0.002 0.000

atensor 12 H
-2.508 1.245 1.028
1.245 1.349 3.487
1.028 3.487 0.855
0.000 0.000 0.000
0.000 0.000 0.000

0.000 -0.001 0.000

atensor 13 C
-0.042 0.225 0.532
0.225 0.656 1.805
0.532 1.805 3.959
0.000 0.001 0.000
0.001 0.004 0.001
-0.001 -0.002 0.000

atensor 14 H
0.248 -2.141 -2.999
-2.141 -1.410 2.054
-2.999 2.054 0.853
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.457 -0.388 -1.552
-0.388 0.157 1.063
-1.552 1.063 3.962
0.003 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.008 2.220 -2.880
2.220 -1.168 -2.216
-2.880 -2.216 0.851
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.417 0.402 -1.491
0.402 0.205 -1.148
-1.491 -1.148 3.967
0.003 0.002 -0.001
0.002 0.001 -0.001
0.002 0.002 0.000

atensor 18 H
-2.361 -1.450 1.217
-1.450 1.201 -3.425
1.217 -3.425 0.851
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 19 C
-0.016 -0.263 0.631
-0.263 0.630 -1.774
0.631 -1.774 3.959
0.000 -0.001 0.000
-0.001 0.004 -0.001
-0.001 0.002 0.000

atensor 20 C
0.723 0.022 1.882
0.022 -0.108 0.051
1.882 0.051 3.961
0.004 0.000 0.001
0.000 0.000 0.000
-0.003 0.000 0.000

atensor 21 H

1.717 0.126 3.634
0.126 -2.868 0.099
3.634 0.099 0.857
0.000 0.000 0.000
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1786.764 15.018 0.214
15.018 -1775.428 -0.093
0.214 -0.093 -159.398
1931.776 0.000 0.002
0.000 1931.775 -0.001
0.002 -0.001 1939.404

orbtensor 2 H
-2.249 5.660 1.070
5.660 -15.828 -2.806
1.070 -2.806 -0.435
28.013 -4.918 -0.920
-4.918 40.101 2.589
-0.920 2.589 25.165

orbtensor 3 C
-211.054 17.487 5.143
17.487 -251.025 -13.872
5.143 -13.872 -64.209
257.442 2.613 -1.179
2.613 251.026 3.316
-1.179 3.316 232.975

orbtensor 4 H
-17.721 -0.515 2.976
-0.515 -0.175 0.118
2.976 0.118 -0.371
41.838 0.426 -2.746
0.426 26.276 -0.075
-2.746 -0.075 25.162

orbtensor 5 C
-255.673 -1.460 14.758
-1.460 -206.886 -0.373
14.758 -0.373 -64.765
250.112 -0.226 -3.517
-0.226 258.380 -0.095
-3.517 -0.095 232.979

orbtensor 6 H
-1.602 -4.822 0.861
-4.822 -16.255 2.843
0.861 2.843 -0.377
27.512 4.228 -0.778
4.228 40.602 -2.635
-0.778 -2.635 25.164

orbtensor 7 C
-208.560 -13.777 3.761
-13.777 -250.788 14.343
3.761 14.343 -64.313
257.710 -2.248 -0.997
-2.248 250.758 -3.374
-0.997 -3.374 232.975

orbtensor 8 H
-12.168 8.298 -2.462
8.298 -5.963 1.727
-2.462 1.727 -0.444

36.865	-7.268	2.266
-7.268	31.246	-1.553
2.266	-1.553	25.162

orbtensor 9 C

-240.288	25.060	-11.858
25.060	-224.261	8.748
-11.858	8.748	-64.501
252.744	3.862	2.901
3.862	255.727	-1.989
2.901	-1.989	232.977

orbtensor 10 H

-11.241	-8.564	-2.331
-8.564	-6.699	-1.814
-2.331	-1.814	-0.483
36.055	7.532	2.177
7.532	32.057	1.675
2.177	1.675	25.163

orbtensor 11 C

-238.014	-24.973	-11.737
-24.973	-225.824	-8.814
-11.737	-8.814	-64.834
253.175	-4.001	2.787
-4.001	255.300	2.146
2.787	2.146	232.976

orbtensor 12 H

-1.599	-4.820	-0.858
-4.820	-16.256	-2.842
-0.858	-2.842	-0.369
27.510	4.226	0.777
4.226	40.603	2.637
0.777	2.637	25.165

orbtensor 13 C

-208.550	-13.766	-3.738
-13.766	-250.790	-14.363
-3.738	-14.363	-64.320
257.710	-2.247	0.989
-2.247	250.757	3.378
0.989	3.378	232.978

orbtensor 14 H

-12.171	8.298	2.463
8.298	-5.961	-1.725
2.463	-1.725	-0.443
36.868	-7.267	-2.268
-7.267	31.243	1.554
-2.268	1.554	25.162

orbtensor 15 C

-240.336	25.060	11.893
25.060	-224.281	-8.764
11.893	-8.764	-64.517
252.746	3.861	-2.905
3.861	255.731	1.990
-2.905	1.990	232.975

orbtensor 16 H

-11.240	-8.567	2.328
-8.567	-6.702	1.815
2.328	1.815	-0.475
36.053	7.533	-2.178
7.533	32.059	-1.675
-2.178	-1.675	25.162

```

orbtensor 17 C
-238.048  -24.975   11.766
-24.975  -225.852   8.795
11.766    8.795  -64.839
253.181  -4.001   -2.792
-4.001   255.300  -2.142
-2.792   -2.142  232.974

```

```

orbtensor 18 H
-2.249    5.662   -1.071
5.662   -15.828   2.800
-1.071    2.800   -0.427
28.014   -4.919   0.919
-4.919   40.101  -2.587
0.919   -2.587   25.165

```

```

orbtensor 19 C
-211.040   17.486   -5.128
17.486  -251.021   13.845
-5.128   13.845  -64.208
257.439    2.615    1.174
2.615   251.027   -3.315
1.174   -3.315   232.972

```

```

orbtensor 20 C
-255.658   -1.453  -14.738
-1.453  -206.858    0.355
-14.738    0.355  -64.769
250.107   -0.229    3.514
-0.229   258.375    0.099
3.514    0.099   232.979

```

```

orbtensor 21 H
-17.721   -0.517   -2.972
-0.517   -0.177   -0.121
-2.972   -0.121   -0.370
41.838    0.428    2.745
0.428   26.277    0.076
2.745    0.076   25.163

```

```

gtensor (ppt)
-0.142    0.000    0.000
0.000   -0.142    0.000
0.000    0.000   -0.164
-0.223   -0.051    0.000
-0.051   -0.244    0.000
0.000    0.000    0.090

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-132.6640	693.78833	126154.80373	-0.13747	126154.66626	126848.45460
2	H	-0.1037	24.92233	24.48719	-0.01566	24.47153	49.39386
3	C	1.5267	71.71833	-1433.84094	-0.11792	-1433.95886	-1362.24053
4	H	-0.1000	25.00300	23.62108	-0.01271	23.60837	48.61137
5	C	1.5283	71.38233	-1435.40627	-0.11588	-1435.52216	-1364.13982
6	H	-0.1020	25.01467	24.09351	-0.00473	24.08877	49.10344
7	C	1.5260	72.59400	-1433.21481	-0.10993	-1433.32475	-1360.73075
8	H	-0.1007	24.89933	23.77856	-0.02060	23.75796	48.65730
9	C	1.5250	70.79933	-1432.27562	-0.12142	-1432.39704	-1361.59770

10	H	-0.1007	24.95067	23.77856	-0.00290	23.77565	48.72632
11	C	1.5287	70.92633	-1435.71934	-0.10868	-1435.82802	-1364.90169
12	H	-0.1013	25.01800	23.93603	-0.00475	23.93128	48.94928
13	C	1.5257	72.59500	-1432.90175	-0.10997	-1433.01171	-1360.41671
14	H	-0.1030	24.89933	24.32972	-0.02061	24.30911	49.20844
15	C	1.5267	70.77267	-1433.84094	-0.12153	-1433.96248	-1363.18981
16	H	-0.1030	24.95233	24.32972	-0.00289	24.32682	49.27916
17	C	1.5310	70.90533	-1437.91080	-0.10876	-1438.01956	-1367.11422
18	H	-0.1030	24.92533	24.32972	-0.01566	24.31406	49.23939
19	C	1.5257	71.72300	-1432.90175	-0.11787	-1433.01961	-1361.29661
20	C	1.5267	71.39200	-1433.84094	-0.11579	-1433.95674	-1362.56474
21	H	-0.0977	25.00333	23.06993	-0.01271	23.05722	48.06055
C Average		1.5270	71.48083	-1434.18532	-0.11477	-1434.30009	-1362.81926
H Average		-0.1015	24.95883	23.97540	-0.01132	23.96408	48.92291

=====

6MnCp2-STO-PBE0-QZ4P-QZ4P

Temperature: 390

Spin: 2.5

atensor 1 Mn

-128.385 0.000 -0.002
0.000 -128.386 0.001
-0.002 0.001 -123.816
-4.115 0.000 0.000
0.000 -4.115 0.000
0.000 0.000 -4.419

atensor 2 H

-2.290 -1.441 -1.218
-1.441 1.252 3.426
-1.218 3.426 0.908
0.000 0.000 0.000
0.000 0.000 0.000
0.000 -0.001 0.000

atensor 3 C

-0.178 -0.261 -0.634
-0.261 0.463 1.782
-0.634 1.782 3.807
0.000 -0.001 0.000
-0.001 0.003 0.001
0.001 -0.002 0.000

atensor 4 H

1.762 0.125 -3.635
0.125 -2.797 -0.099
-3.635 -0.099 0.911
0.000 0.000 0.000
0.000 0.001 0.000
0.001 0.000 0.000

atensor 5 C

0.555 0.022 -1.890
0.022 -0.270 -0.052
-1.890 -0.052 3.810
0.004 0.000 -0.001
0.000 0.000 0.000
0.003 0.000 0.000

atensor 6 H

-2.436 1.239 -1.029
1.239 1.399 -3.488
-1.029 -3.488 0.910
0.001 0.000 0.000

0.000 0.000 0.000
0.000 0.001 0.000

atensor 7 C
-0.205 0.224 -0.535
0.224 0.489 -1.814
-0.535 -1.814 3.805
0.000 0.001 0.000
0.001 0.004 -0.001
0.001 0.002 0.000

atensor 8 H
0.306 -2.130 3.000
-2.130 -1.341 -2.056
3.000 -2.056 0.911
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 9 C
0.290 -0.385 1.560
-0.385 -0.007 -1.070
1.560 -1.070 3.804
0.003 -0.002 0.001
-0.002 0.001 -0.001
-0.002 0.001 0.000

atensor 10 H
0.067 2.207 2.883
2.207 -1.104 2.217
2.883 2.217 0.910
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 11 C
0.250 0.399 1.499
0.399 0.038 1.154
1.499 1.154 3.809
0.002 0.002 0.001
0.002 0.001 0.001
-0.002 -0.002 0.000

atensor 12 H
-2.436 1.238 1.028
1.238 1.400 3.489
1.028 3.489 0.912
0.001 0.000 0.000
0.000 0.000 0.000
0.000 -0.001 0.000

atensor 13 C
-0.205 0.224 0.535
0.224 0.489 1.814
0.535 1.814 3.805
0.000 0.001 0.000
0.001 0.004 0.001
-0.001 -0.002 0.000

atensor 14 H
0.304 -2.129 -3.000
-2.129 -1.344 2.055
-3.000 2.055 0.909
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.000 0.000

atensor 15 C
0.292 -0.385 -1.560
-0.385 -0.006 1.069
-1.560 1.069 3.808
0.003 -0.002 -0.001
-0.002 0.001 0.001
0.002 -0.001 0.000

atensor 16 H
0.065 2.207 -2.882
2.207 -1.105 -2.217
-2.882 -2.217 0.907
0.000 -0.001 0.000
-0.001 0.000 0.000
0.000 0.000 0.000

atensor 17 C
0.251 0.399 -1.499
0.399 0.040 -1.154
-1.499 -1.154 3.812
0.002 0.002 -0.001
0.002 0.001 -0.001
0.002 0.002 0.000

atensor 18 H
-2.289 -1.442 1.218
-1.442 1.253 -3.427
1.218 -3.427 0.909
0.000 0.000 0.000
0.000 0.000 0.000
0.000 0.001 0.000

atensor 19 C
-0.179 -0.261 0.634
-0.261 0.462 -1.782
0.634 -1.782 3.804
0.000 -0.001 0.000
-0.001 0.003 -0.001
-0.001 0.002 0.000

atensor 20 C
0.554 0.022 1.891
0.022 -0.271 0.051
1.891 0.051 3.805
0.004 0.000 0.001
0.000 0.000 0.000
-0.003 0.000 0.000

atensor 21 H
1.764 0.125 3.636
0.125 -2.795 0.099
3.636 0.099 0.914
0.000 0.000 0.000
0.000 0.001 0.000
-0.001 0.000 0.000

orbtensor 1 Mn
-1804.654 1.879 0.223
1.879 -1822.179 -0.136
0.223 -0.136 -20.823
1926.029 0.000 0.001
0.000 1926.031 -0.001
0.001 -0.001 1943.375

orbtensor 2 H
0.802 6.987 0.723
6.987 -16.183 -1.851

0.723	-1.851	1.532
24.936	-6.265	-0.681
-6.265	40.336	1.915
-0.681	1.915	22.988

orbtensor 3 C

-214.669	19.317	6.585
19.317	-258.443	-19.300
6.585	-19.300	-69.990
254.417	-0.038	-0.900
-0.038	254.518	2.528
-0.900	2.528	230.575

orbtensor 4 H

-18.870	-0.559	2.123
-0.559	3.215	0.011
2.123	0.011	1.522
42.548	0.543	-2.033
0.543	22.725	-0.056
-2.033	-0.056	22.986

orbtensor 5 C

-268.731	-1.731	20.334
-1.731	-207.180	0.950
20.334	0.950	-69.998
254.538	0.004	-2.684
0.004	254.411	-0.073
-2.684	-0.073	230.578

orbtensor 6 H

1.395	-5.914	0.566
-5.914	-17.076	1.883
0.566	1.883	1.401
24.299	5.386	-0.575
5.386	40.974	-1.950
-0.575	-1.950	22.988

orbtensor 7 C

-210.882	-15.243	4.853
-15.243	-263.982	19.057
4.853	19.057	-69.599
254.411	0.035	-0.761
0.035	254.518	-2.573
-0.761	-2.573	230.572

orbtensor 8 H

-11.743	10.236	-1.808
10.236	-3.793	1.157
-1.808	1.157	1.341
36.214	-9.259	1.676
-9.259	29.054	-1.149
1.676	-1.149	22.986

orbtensor 9 C

-246.992	27.847	-15.463
27.847	-226.353	10.033
-15.463	10.033	-69.315
254.490	-0.061	2.210
-0.061	254.441	-1.516
2.210	-1.516	230.576

orbtensor 10 H

-10.630	-10.676	-1.707
-10.676	-5.044	-1.213
-1.707	-1.213	1.437
35.182	9.595	1.611
9.595	30.087	1.239

```

1.611      1.239      22.987

orbtensor 11 C
-245.009  -30.259  -15.266
-30.259  -230.963  -12.101
-15.266  -12.101  -69.354
254.483   0.063   2.125
0.063  254.448   1.636
2.125   1.636  230.575

orbtensor 12 H
1.397   -5.911   -0.567
-5.911  -17.076   -1.884
-0.567  -1.884    1.400
24.297   5.384    0.575
5.384   40.975    1.951
0.575   1.951   22.988

orbtensor 13 C
-210.865  -15.231   -4.828
-15.231  -263.976  -19.069
-4.828  -19.069  -69.597
254.410   0.035   0.755
0.035  254.517   2.576
0.755   2.576  230.574

orbtensor 14 H
-11.747   10.235    1.810
10.235   -3.790   -1.163
1.810   -1.163    1.339
36.217   -9.258   -1.679
-9.258   29.052    1.150
-1.679    1.150   22.986

orbtensor 15 C
-247.018   27.848   15.489
27.848  -226.341  -10.048
15.489  -10.048  -69.307
254.490   -0.060   -2.216
-0.060  254.442    1.518
-2.216   1.518  230.575

orbtensor 16 H
-10.627  -10.678    1.708
-10.678   -5.048    1.214
1.708    1.214    1.436
35.179    9.596   -1.611
9.596   30.091   -1.239
-1.611   -1.239   22.986

orbtensor 17 C
-245.007  -30.265   15.252
-30.265  -230.996   12.090
15.252   12.090  -69.339
254.482   0.064   -2.129
0.064  254.452   -1.633
-2.129  -1.633  230.573

orbtensor 18 H
0.800    6.990   -0.720
6.990  -16.181    1.849
-0.720   1.849    1.532
24.938   -6.267    0.680
-6.267   40.334   -1.913
0.680   -1.913   22.987

orbtensor 19 C

```

```

-214.672  19.337  -6.565
19.337 -258.438  19.268
-6.565  19.268  -69.965
254.416  -0.040  0.895
-0.040  254.518  -2.526
0.895  -2.526  230.573

```

```

orbtensor 20 C
-268.722  -1.739  -20.278
-1.739 -207.164  -0.973
-20.278  -0.973  -69.986
254.536  0.004  2.679
0.004  254.409  0.076
2.679  0.076  230.579

```

```

orbtensor 21 H
-18.869  -0.563  -2.121
-0.563  3.215  -0.011
-2.121  -0.011  1.520
42.548  0.546  2.030
0.546  22.725  0.056
2.030  0.056  22.986

```

```

gtensor (ppt)
-0.146  0.000  0.000
0.000  -0.146  0.000
0.000  0.000  -0.163
-0.254  -0.009  0.000
-0.009  -0.166  0.000
0.000  0.000  -0.360

```

```

averaging
C Average:3,5,7,9,11,13,15,17,19,20
H Average:2,4,6,8,10,12,14,16,18,21

```

Final results. Shifts and Shieldings in ppm.
Elements for which I don't have the nuclear g factor may show "inf" or "nan"

#	El	Aiso (MHz)	Orb Shielding	FC Shield	PC Shield	FC+PC Shield	Total**
1	Mn	-131.0787	715.92633	124638.74635	0.07520	124638.82155	125354.74788
2	H	-0.0433	24.80367	10.23510	-0.00090	10.23420	35.03787
3	C	1.3650	65.46933	-1281.91656	0.05860	-1281.85796	-1216.38863
4	H	-0.0410	24.70867	9.68398	0.01423	9.69821	34.40688
5	C	1.3663	64.53933	-1283.16874	0.06958	-1283.09916	-1218.55983
6	H	-0.0420	24.66033	9.92018	0.00050	9.92067	34.58101
7	C	1.3643	65.01267	-1281.29047	0.05957	-1281.23091	-1216.21824
8	H	-0.0413	24.68633	9.76272	0.00760	9.77031	34.45665
9	C	1.3637	65.61567	-1280.66438	0.06470	-1280.59969	-1214.98402
10	H	-0.0423	24.67300	9.99891	0.00984	10.00875	34.68175
11	C	1.3667	64.72667	-1283.48178	0.06637	-1283.41541	-1218.68874
12	H	-0.0410	24.66033	9.68398	0.00050	9.68448	34.34482
13	C	1.3643	65.02100	-1281.29047	0.05957	-1281.23091	-1216.20991
14	H	-0.0437	24.68567	10.31384	0.00760	10.32144	35.00710
15	C	1.3660	65.61367	-1282.85569	0.06475	-1282.79095	-1217.17728
16	H	-0.0443	24.67233	10.47130	0.00983	10.48113	35.15347
17	C	1.3687	64.72167	-1285.36005	0.06639	-1285.29366	-1220.57199
18	H	-0.0423	24.80333	9.99891	-0.00090	9.99801	34.80134
19	C	1.3633	65.47733	-1280.35134	0.05857	-1280.29277	-1214.81544
20	C	1.3640	64.55067	-1280.97743	0.06951	-1280.90792	-1216.35725
21	H	-0.0387	24.70833	9.13286	0.01423	9.14710	33.85543
C Average		1.3652	65.07480	-1282.13569	0.06376	-1282.07193	-1216.99713
H Average		-0.0420	24.70620	9.92018	0.00625	9.92643	34.63263

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