Group 13-derived radicals from α-diimines via hydro- and carboalumination reactions†

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EPR spectra

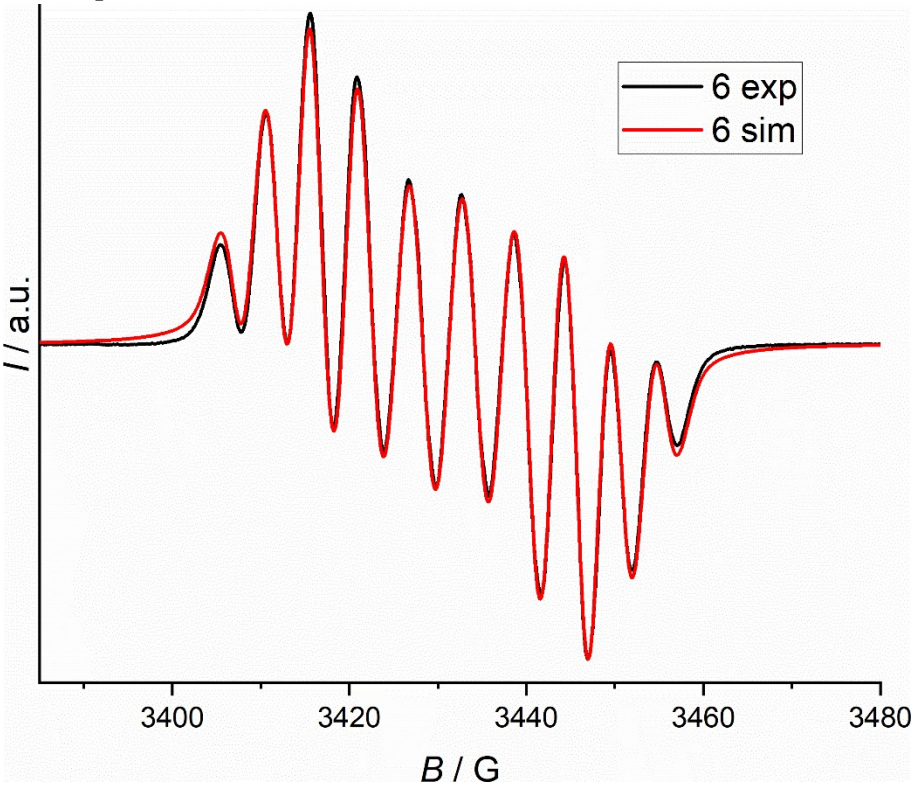

Figure 1: EPR spectrum of **6** (black) and simulation (red).

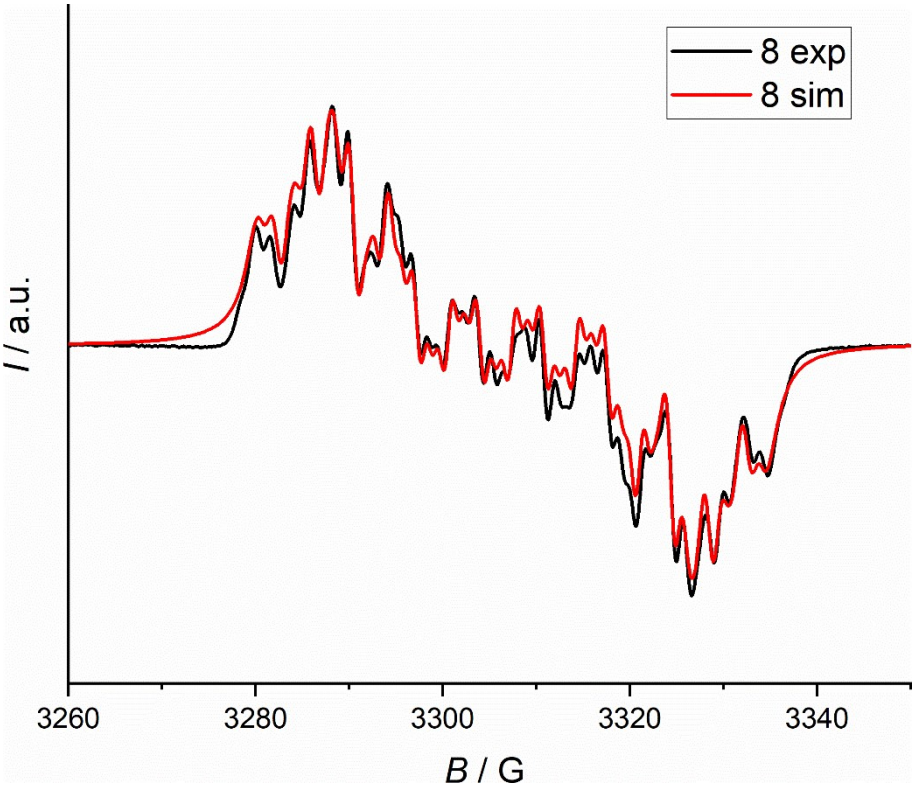

Figure 2: EPR spectrum of **8** (black) and simulation (red).

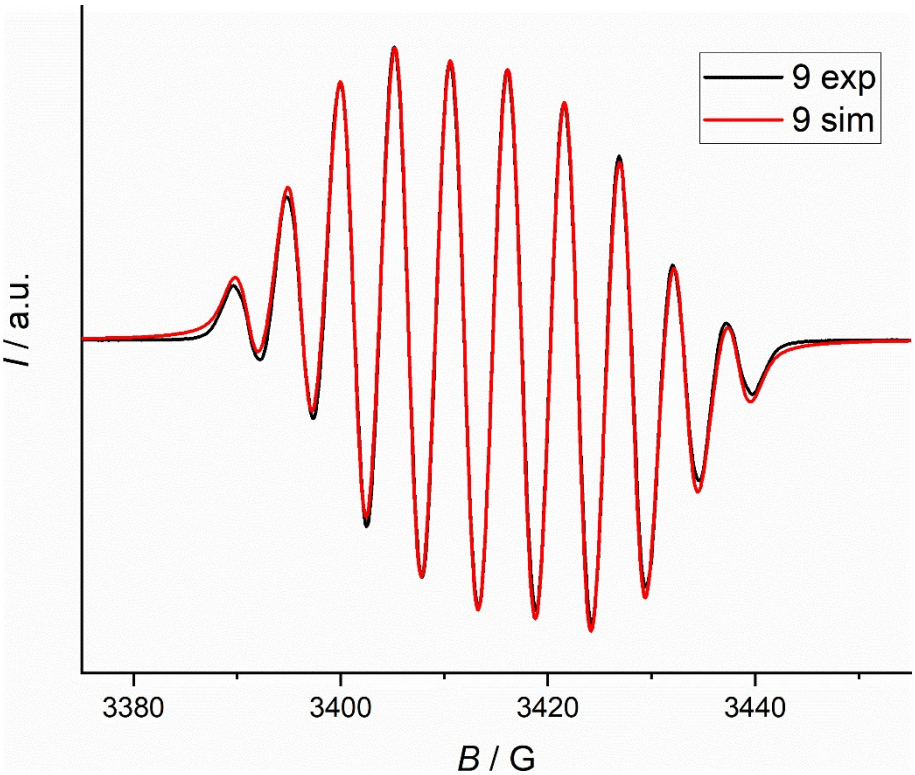

Figure 3: EPR spectrum of **9** (black) and simulation (red).

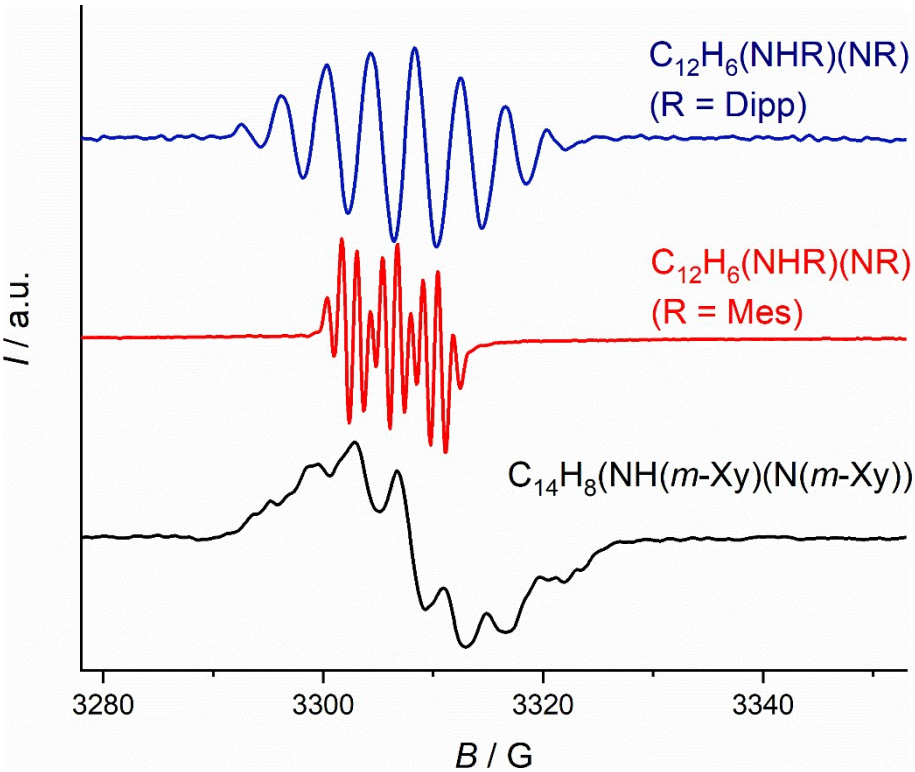

Figure 4: Experimental EPR spectra of the ligand radicals $C_{12}H_6$(NHR)(NR) (R = Dipp (blue), Mes (red)) and $C_{14}H_8$(NH(*m*-Xy)(N(*m*-Xy)) (black).

NMR spectra

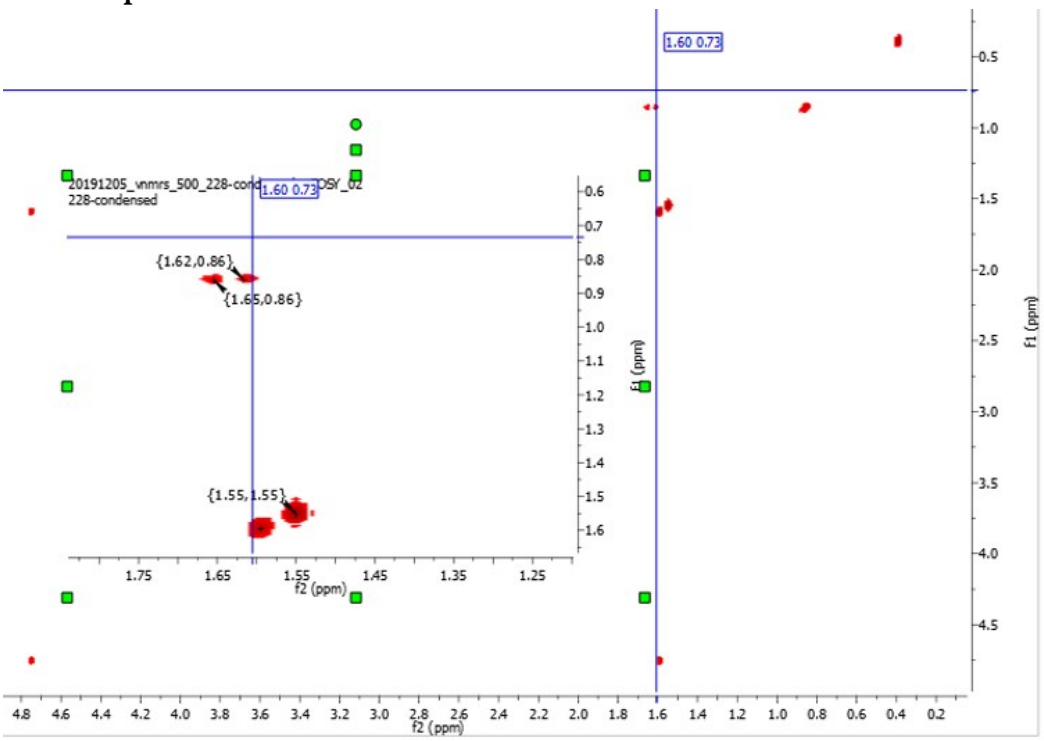

Figure 5: COSY{^{1}H,^{1}H}(500 MHz) spectrum of the reaction AliBu$_3$ with $C_{14}H_8$(N(*m*-Xy)$_2$, iso-butane is found with cross peak doublet at (1.63, 0.86), which is the consistent as described in the literature.[1]

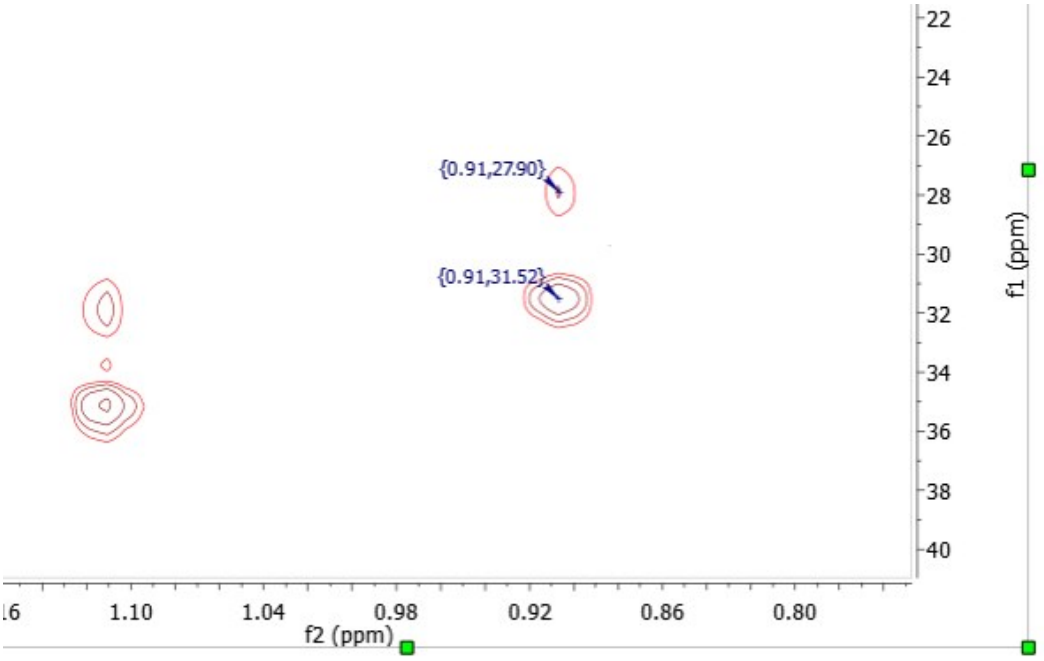

Figure 6: HMBC{^{1}H,^{13}C}(500 MHz) spectrum of the reaction AliNp$_3$ with $C_{14}H_8$(N(*m*-Xy)$_2$, neo-pentane is found with cross peaks at (0.91, 27.9 ((H$_3$C)$_3$-**C**-C**H**$_3$)) and (0.91, 31.5(H$_3$**C**)$_3$-C-C**H**$_3$)), which is the consistent as described in the literature.[2]

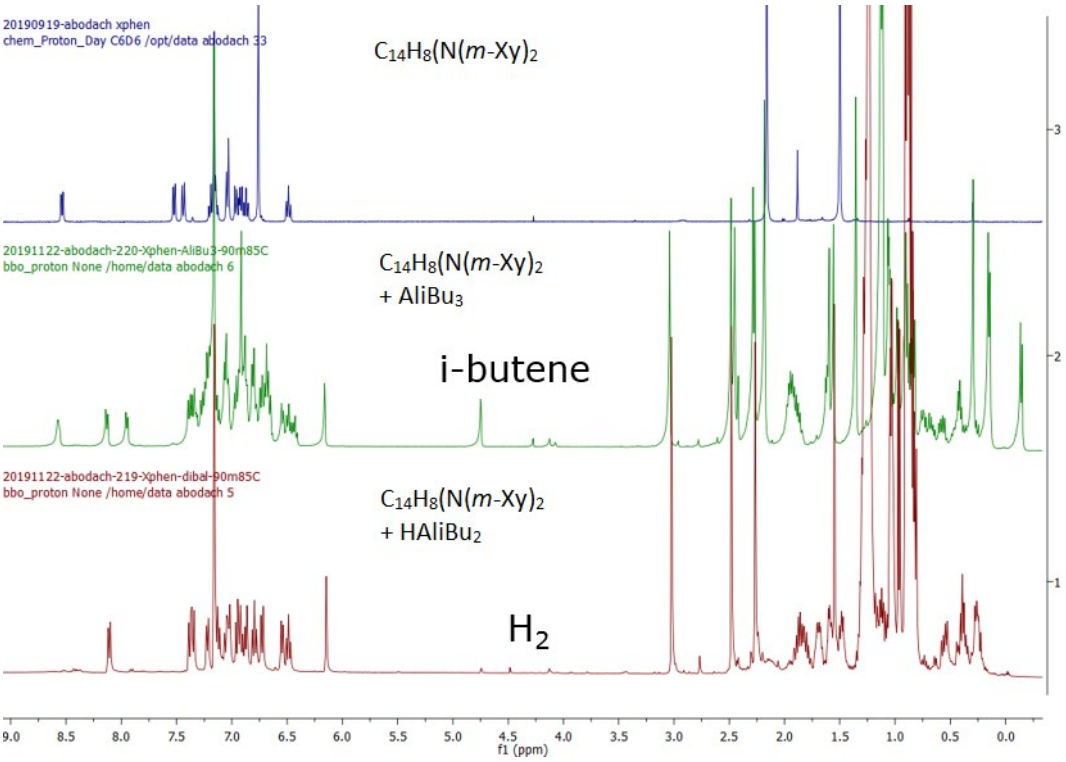

Figure 7: ^{1}H(400 MHz) NMR sprectra of $C_{14}H_8(N(m\text{-}Xy)_2$, the reaction of $C_{14}H_8(N(m\text{-}Xy)_2$ with $AliBu_3$ and the reaction of $C_{14}H_8(N(m\text{-}Xy)_2$ with H $AliBu_2$. H_2 and iso-butene were found consistent with literature.[3, 4]

Crystallographic content

Table 1: Selected crystallograohic data

	4	**5**	**9**	**10**	**12**	**13**
CCDC No	2016535	2014670	2014632	2014630	2014631	2014629
empirical formula	$C_{39}H_{53}Al_2$	$C_{44}H_{59}AlN_2$	$C_{46}H_{62}AlN_2$	$C_{40}H_{50}AlN_2$	$C_{42}H_{53}AlN_2$	$C_{32}H_8BF_{15}O$
formula weight	575.77	642.91	669.95	585.80	559.67	720.19
crystal system	Tetragonal	Triclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P\bar{4}2_1c$	P -1	P 1 21/n 1	C 1 2/c 1	P 1 21/n 1	P21/c
a (Å)	22.951(2)	10.512(2)	15.119(3)	28.0580(14)	11.976(2)	10.5437(15)
b (Å)	22.951(2)	10.892(2)	16.789(3)	11.3822(6)	19.461(4)	9.6540(15)
c (Å)	14.843(2)	18.272(4)	16.015(3)	22.1186(10)	16.046(3)	27.089(4)
α (°)	90	100.78(3)	90	90	90	90
β (°)	90	103.05(3)	100.62(3)	103.030(3)	103.55(3)	97.184(9)
γ (°)	90	102.43(3)	90	90	90	90
V (Å^3)	7818.6(19)	1928.1(8)	3995.6(14)	6882.0(6)	3635.7(13)	2735.7(7)

Z	8	2	4	8	4	4
D_{calc} ($g \cdot cm^{-3}$)	1.051	1.107	1.114	1.131	1.022	1.749
μ (mm^{-1})	0.100	0.084	0.084	0.088	0.083	0.178
θ_{min} (°)	2.745	1.976	2.426	2.229	2.038	2.242
θ_{max} (°)	27.499	25.027	25.027	27.891	25.00	27.721
reflections measured	89495	13678	100180	66293	57225	45615
unique reflections	8979	6393	6997	8191	6390	6392
R_{int}	0.0685	0.1268	0.1233	0.1013	0.2110	0.0610
No. of parameters	419	437	472	400	416	451
R_1	0.0562	0.0615	0.0526	0.0580	0.0650	0.0871
wR_2	0.1434	0.1671	0.1553	0.1420	0.1432	0.1056
GOF on F^2	1.110	0.965	0.986	1.011	1.0546	1.009

Computational results

DFT survey

The DFT survey was conducted in two parts: First the crystal structure of a known compound should be reproduced on an acceptable level, *Table 2*. Second, based on the single crystal and calculated structures a suitable level of theory for the prediction of the EPR spectra was tested, .

Table 2: DFT survey to describe the molecular structure, based on the single crystal (SC) structure of **10**, *d* refers to the deviation from the SC structure, selected bond lengths in Å, selected bond angles in °, sums gives below.

parameter	**SC**	SC-esd	**6-31+G****	*d*	**cc-pVDZ**	*d*	**6311G**	*d*
Al-N1	1.9615	0.0019	1.984	0.0225	1.999	0.0375	1.999	0.0375
Al-N2	1.9738	0.0016	1.988	0.0142	2.015	0.0412	1.999	0.0252
N-Al-N	84.95	0.11	84.93	0.02	84.39	0.56	84.62	-0.33
C-C (Ace)	1.446	0.004	1.435	0.011	1.437	0.009	1.437	-0.009
Al-Ca	1.986	0.002	1.993	0.007	1.998	0.012	2.006	0.02
Al-Cb	1.988	0.003	1.999	0.011	2.004	0.016	2.006	0.018
C1-N1	1.333	0.003	1.342	0.009	1.343	0.01	1.348	0.015
C2-N2	1.32	0.003	1.34	0.02	1.341	0.021	1.348	0.028
C1-naph	1.47	0.004	1.466	0.004	1.468	0.002	1.468	-0.002
C2-naph	1.469	0.003	1.469	0	1.47	0.001	1.468	-0.001
N1-C1-C2	117.2	0.3	117.88	0.68	118	0.8	117.75	0.55
C1-C2-N2	117.2	0.3	117.82	0.62	117.95	0.75	117.75	0.55
C1-N1-Al	110.13	0.18	109.85	0.28	110.02	0.11	109.94	-0.19
C2-N2-Al	110.25	0.18	109.48	0.77	109.59	0.66	109.94	-0.31
	SUM	1.0955		2.4687		3.0297		0.4017
	SUM-length	0.0255		0.0987		0.1497		0.1317
	SUM-angles	0.964		2.361		2.329		0.591

Table 3: DFT survey to describe the hyperfine couplings of the EPR spectra, based on the single crystal (SC) structure of **10**, as well as calculated structures.

structure	exp	b3lyp/631-G**	b3lyp/cc-pVDZ	SC	SC	SC	6311G	6311G
EPR	exp	UM062X def2TZVP	UM062X def2TZVP	UM062X def2TZVP	UB3LYP def2TZVP	UPBE def2TZVP	UM062X def2TZVP	UB3LYP def2TZVP
Al	6.029	7.317	7.259	7.008	6.651	6.65	7.317	6.836
N	4.507	5.116	4.988	5.024	3.334	3.33	5.333	3.597
	4.507	5.182	5.063	4.848	3.263	3.26	5.334	
relative		1.21	1.20	1.16	1.10	1.10	1.21	1.13
		1.14	1.11	1.11	0.74	0.74	1.18	0.80

Cartesian coordinates

Compound **6**

C	2.32934	4.64706	-0.12749
C	2.34225	3.22722	-0.02000
C	1.16581	5.37136	-0.32573
H	3.28138	2.70080	0.11767
C	1.13910	2.54842	-0.10246
C	-0.05453	3.30393	-0.29605
C	-0.08789	4.69834	-0.42349
C	-1.37011	5.28193	-0.64593
C	-1.20850	2.47048	-0.36408
C	-2.43748	3.06228	-0.59385
C	-2.49471	4.47822	-0.73235
C	-0.71702	1.10212	-0.17898
C	0.71268	1.14606	-0.05606
N	-1.29989	-0.09588	-0.09188
N	1.36182	-0.02111	0.03526
H	-1.45964	6.36078	-0.75350
H	-3.46321	4.93980	-0.90962
H	-3.34459	2.47038	-0.66467
C	2.79492	-0.01663	0.09606
C	-2.72356	-0.23947	-0.12527
C	-3.29162	-0.71793	-1.33588
C	-3.52651	0.01762	1.01170
C	-4.89612	-0.28805	0.90622
C	-5.46356	-0.78066	-0.26099
C	-4.66286	-0.97698	-1.38366
C	3.39004	-0.05930	1.38153
C	3.58738	0.05360	-1.07564
C	4.78380	-0.05347	1.48528
C	5.58299	0.00892	0.34790
C	4.98312	0.06877	-0.90398
H	6.66682	0.02286	0.43618
H	5.24563	-0.08018	2.46924
H	5.61208	0.13250	-1.79031
C	2.54995	-0.04798	2.65443
C	2.87394	-1.23753	3.57365
H	3.90273	-1.19252	3.95113
H	2.20275	-1.24165	4.44100
H	2.74831	-2.18940	3.04635
C	2.69909	1.29456	3.39500
H	2.05330	1.31808	4.28146
H	2.42063	2.13335	2.74704
H	3.73294	1.45360	3.72661
H	1.50000	-0.13685	2.36889
C	3.13899	0.10703	-2.55002
C	1.73249	0.60952	-2.90816
C	3.39704	-1.24708	-3.24666
H	3.83371	0.82613	-3.00957
H	2.69075	-2.00543	-2.89941
H	4.40958	-1.61743	-3.05383
H	3.27158	-1.14473	-4.33169

C	-3.11946	0.61379	2.37595
C	-1.63958	0.70307	2.77896
H	-3.59313	-0.05324	3.11199
C	-3.76135	2.00871	2.56132
C	-2.43874	-0.86773	-2.59191
C	-2.49004	0.42779	-3.42613
C	-2.81102	-2.08827	-3.44691
H	-1.40101	-1.00166	-2.27905
H	-3.78824	-1.97128	-3.93136
H	-2.83881	-3.00387	-2.84583
H	-2.06925	-2.22653	-4.24197
H	-3.51417	0.63103	-3.76468
H	-1.84840	0.34236	-4.31194
H	-2.15094	1.29040	-2.84302
H	-3.30090	2.73660	1.88492
H	-3.60551	2.36072	3.58850
H	-4.83845	2.00141	2.36580
H	-1.09904	-0.22666	2.61402
H	-1.58650	0.93645	3.84940
H	-1.11432	1.50341	2.25045
H	-5.52917	-0.13647	1.77845
H	-6.52640	-1.00803	-0.29770
H	3.27649	5.17679	-0.05724
H	1.20371	6.45527	-0.41074
H	0.94585	-0.06316	-2.56015
H	1.65253	0.67089	-4.00050
H	1.53735	1.60739	-2.50835
Al	0.06532	-1.52072	0.14043
C	0.32303	-2.80284	-1.35881
C	-0.17951	-2.47010	1.88170
H	0.19002	-1.89891	2.74521
C	-1.61181	-2.96734	2.20429
H	0.47736	-3.35601	1.83841
H	-0.66253	-3.16625	-1.69031
C	1.18163	-4.03960	-0.99140
H	0.75212	-2.31650	-2.24753
H	-2.26096	-2.09224	2.35148
C	-1.63448	-3.77727	3.51020
C	-2.22583	-3.78577	1.05768
H	-2.35995	-3.18341	0.15083
H	-3.21415	-4.17489	1.33300
H	-1.58796	-4.64200	0.80071
H	-1.23001	-3.19130	4.34508
H	-1.01932	-4.68258	3.41338
H	-2.65227	-4.09165	3.77865
C	1.36870	-4.97097	-2.19990
H	0.63415	-4.60663	-0.22254
C	2.54792	-3.66747	-0.39002
H	0.40053	-5.27551	-2.61622
H	1.92543	-5.88009	-1.93491
H	1.92566	-4.46107	-2.99824
H	3.15529	-3.09009	-1.09543

H	3.11965	-4.56434	-0.11898
H	2.44974	-3.05943	0.51874
H	-5.10935	-1.34073	-2.30474

Compound **7**

C	-2.42253	-4.60167	0.21980
C	-2.39953	-3.17810	0.21601
C	-1.17728	-2.53936	0.10414
C	0.00012	-3.33626	0.00003
C	-1.27353	-5.36796	0.11560
C	0.00017	-4.73668	0.00007
C	1.17747	-2.53929	-0.10411
C	2.39976	-3.17795	-0.21594
C	1.27390	-5.36788	-0.11543
C	2.42286	-4.60152	-0.21965
C	-0.71500	-1.14906	0.06510
C	0.71510	-1.14903	-0.06513
N	1.33208	0.03799	-0.13206
N	-1.33204	0.03792	0.13203
C	2.76128	0.08657	-0.18048
C	-2.76124	0.08643	0.18055
C	3.49961	-0.04582	1.01143
C	3.40741	0.25846	-1.41775
C	4.80481	0.32871	-1.43599
C	5.56573	0.22794	-0.26725
C	4.89359	0.03140	0.94407
C	-3.49966	-0.04626	-1.01128
C	-3.40728	0.25857	1.41783
C	-4.80468	0.32876	1.43617
C	-4.89364	0.03089	-0.94381
C	-5.56570	0.22767	0.26752
H	3.38512	-5.10069	-0.30712
H	3.32639	-2.61802	-0.29738
H	1.33851	-6.45392	-0.12091
H	-1.33807	-6.45400	0.12114
H	-3.38476	-5.10089	0.30729
H	-3.32620	-2.61822	0.29744
H	-5.46930	-0.06565	-1.86345
H	-5.31038	0.45907	2.39204
H	5.31059	0.45883	-2.39185
H	5.46918	-0.06491	1.86377
C	7.07047	0.35145	-0.30686
H	7.47575	0.02267	-1.27033
H	7.54349	-0.24341	0.48267
H	7.38326	1.39437	-0.16001
C	2.61021	0.31886	-2.69755
H	1.95316	-0.55430	-2.79194
H	3.27065	0.34599	-3.56991
H	1.96477	1.20273	-2.73085
C	2.79892	-0.29635	2.32361
H	1.99133	0.42409	2.48611
H	3.49853	-0.22931	3.16251
H	2.34431	-1.29544	2.34071
C	-2.79909	-0.29703	-2.32347
H	-1.99146	0.42334	-2.48614
H	-3.49876	-0.23006	-3.16234

H	-2.34455	-1.29614	-2.34046
C	-2.60997	0.31939	2.69754
H	-1.95260	-0.55352	2.79198
H	-3.27035	0.34641	3.56995
H	-1.96484	1.20350	2.73068
C	-7.07044	0.35111	0.30723
H	-7.54349	-0.24393	-0.48215
H	-7.38329	1.39398	0.16020
H	-7.47561	0.02250	1.27080
Al	-0.00002	1.49483	-0.00008
C	-0.12437	2.59378	-1.65431
C	0.12416	2.59407	1.65396
H	0.34354	1.98654	2.54794
H	-0.89413	2.98688	1.82725
C	1.09454	3.79897	1.61990
H	0.89384	2.98666	-1.82784
C	-1.09488	3.79859	-1.62034
H	-0.34384	1.98604	-2.54811
H	-0.83776	4.42312	-0.75007
C	-2.55754	3.36152	-1.45185
C	-0.94562	4.67515	-2.87428
C	2.55728	3.36201	1.45174
C	0.94498	4.67579	2.87361
H	0.83750	4.42328	0.74944
H	-2.71864	2.79368	-0.52761
H	-2.87125	2.71911	-2.28524
H	-3.23289	4.22635	-1.42947
H	1.19769	4.10151	3.77595
H	-0.08606	5.03301	2.98712
H	1.60519	5.55312	2.84085
H	0.08536	5.03244	-2.98804
H	-1.60592	5.55241	-2.84161
H	-1.19842	4.10064	-3.77645
H	2.87092	2.71982	2.28532
H	3.23255	4.22691	1.42928
H	2.71857	2.79398	0.52765

Compound **8**

C	-2.63395	2.48488	0.09162
C	-1.41648	3.27562	-0.10208
C	-2.53970	1.07684	0.27249
C	-1.24858	0.42017	0.16170
C	-0.02939	1.20981	0.13831
C	-0.13088	2.66343	0.02075
C	-1.48003	4.66173	-0.35203
C	-0.34237	5.44989	-0.42293
C	1.01185	3.50071	-0.00912
C	0.91366	4.86505	-0.22417
C	-3.70980	0.34820	0.59664
C	-4.94399	0.96700	0.68167
C	-5.04701	2.34646	0.45360
C	-3.90728	3.08610	0.17920
H	-2.44381	5.13722	-0.49655
H	-0.43186	6.51554	-0.61888
H	1.81558	5.47136	-0.24562
H	1.99353	3.07516	0.12919
H	-4.00922	4.15900	0.05942
H	-6.01180	2.84371	0.51651
H	-5.82498	0.38310	0.93545
H	-3.64044	-0.71332	0.79107
N	1.10574	0.47571	0.14670
N	-1.07750	-0.92559	0.08426
C	2.41961	0.91643	-0.22006
C	-2.02953	-1.80341	-0.52390
C	-2.47203	-2.94406	0.18205
C	-3.34604	-3.83646	-0.44676
C	-3.77715	-3.62186	-1.75352
C	-3.32703	-2.50010	-2.44481
C	-2.45294	-1.57909	-1.85660
C	2.74274	1.01736	-1.59101
C	3.39181	1.16212	0.77163
C	4.69987	1.45783	0.36850
C	5.04115	1.52410	-0.98035
C	4.06045	1.31923	-1.94910
C	1.68563	0.82437	-2.64791
H	1.24247	-0.17471	-2.58351
H	2.10728	0.94425	-3.65030
H	0.87214	1.55096	-2.53235
C	3.01750	1.19869	2.23135
H	2.76144	0.20803	2.61496
H	2.13994	1.83700	2.39059
H	3.84073	1.59350	2.83475
C	-2.04517	-3.18522	1.60748
H	-2.10262	-2.26766	2.20246
H	-1.00746	-3.53468	1.66626
H	-2.67460	-3.94535	2.08083
C	-1.98912	-0.38850	-2.65915
H	-2.13856	-0.56462	-3.72905
H	-0.92973	-0.17978	-2.49248

H	-2.54153	0.52062	-2.38958
H	4.31514	1.39102	-3.00444
H	6.06290	1.74979	-1.27557
H	5.45330	1.64900	1.12984
H	-3.69396	-4.70737	0.10512
H	-4.45559	-4.32479	-2.23069
H	-3.64985	-2.33116	-3.47028
Al	0.77835	-1.44528	0.35871
C	1.33759	-2.09537	2.16119
C	1.36902	-2.59490	-1.15113
C	0.59178	-1.83106	3.49379
C	2.83860	-2.57989	-1.63218
C	3.83375	-2.70698	-0.46883
C	3.09292	-3.67665	-2.67861
C	-0.06339	-0.44405	3.58855
C	1.51693	-2.06717	4.69949
H	-0.22023	-2.56744	3.56910
H	2.33557	-1.33369	4.70847
H	1.97041	-3.06522	4.66047
H	0.97889	-1.97509	5.65268
H	0.68004	0.35791	3.52669
H	-0.59411	-0.32397	4.54216
H	-0.78824	-0.28445	2.78296
H	2.36997	-1.71454	2.25431
H	1.48847	-3.18407	2.06398
H	2.94467	-4.67249	-2.23818
H	4.11725	-3.63513	-3.07328
H	2.40017	-3.58432	-3.52444
H	3.77816	-1.84333	0.20547
H	4.86778	-2.76918	-0.83126
H	3.63157	-3.60964	0.12382
H	0.70533	-2.43265	-2.01640
H	1.13507	-3.62504	-0.82193
H	3.03685	-1.61314	-2.11626

Compound **9**

C	4.56708	2.80545	-0.20771
C	3.84316	1.58421	-0.09848
C	3.94669	4.02773	-0.40392
H	4.37598	0.64964	0.04375
C	2.46222	1.62426	-0.18316
C	1.83358	2.88925	-0.37086
C	2.52567	4.10087	-0.49524
C	1.72920	5.26602	-0.70095
C	0.41458	2.77578	-0.42255
C	-0.33291	3.92160	-0.62730
C	0.34952	5.16294	-0.76745
C	0.12380	1.35321	-0.24109
C	1.36867	0.64253	-0.13263
N	-1.00670	0.64913	-0.13939
N	1.32179	-0.68802	-0.00880
H	2.21072	6.23570	-0.80717
H	-0.24185	6.06147	-0.92672
H	-1.41701	3.88775	-0.66631
C	2.55953	-1.40584	0.16424
C	-2.28865	1.28139	0.00213
C	-3.17155	1.34376	-1.10824
C	-2.71855	1.71554	1.28892
C	-4.08189	1.99965	1.46045
C	-4.99481	1.89861	0.41820
C	-4.52777	1.60735	-0.85552
C	2.97390	-1.66749	1.49764
C	3.37014	-1.79627	-0.93224
C	4.17558	-2.34493	1.72125
C	4.97495	-2.75236	0.65877
C	4.57050	-2.46922	-0.63871
H	5.91275	-3.27230	0.84008
H	4.49680	-2.53583	2.74191
H	5.20614	-2.77130	-1.46920
C	2.18924	-1.15291	2.69849
C	1.94743	-2.23482	3.76429
H	2.87745	-2.53963	4.25918
H	1.27478	-1.85169	4.54138
H	1.48762	-3.12836	3.32878
C	2.88248	0.07934	3.31122
H	2.29378	0.47489	4.14795
H	3.00093	0.87726	2.57078
H	3.87968	-0.17972	3.68931
H	1.21367	-0.82439	2.34275
C	3.13693	-1.59850	-2.44236
C	2.27989	-0.42207	-2.92829
C	2.67929	-2.92121	-3.09523
H	4.14466	-1.40017	-2.83705
H	1.67474	-3.19919	-2.76979
H	3.35641	-3.74418	-2.84109
H	2.66244	-2.81868	-4.18746
C	-1.86909	2.01623	2.54268

C	-0.54055	1.28864	2.78697
H	-2.51937	1.73529	3.38225
C	-1.64991	3.54118	2.66587
C	-2.81366	1.27927	-2.60638
C	-1.42036	0.81523	-3.04211
C	-3.06058	2.67531	-3.23096
H	-3.53937	0.58702	-3.05757
H	-2.34327	3.40190	-2.82957
H	-4.06767	3.05493	-3.03426
H	-2.91885	2.63353	-4.31789
H	-0.64193	1.52194	-2.73898
H	-1.39640	0.75307	-4.13713
H	-1.16651	-0.16435	-2.64890
H	-0.97812	3.90532	1.88267
H	-1.19439	3.77788	3.63563
H	-2.59353	4.09197	2.58764
H	-0.61865	0.21816	2.60277
H	-0.25410	1.42677	3.83662
H	0.27457	1.68686	2.17916
H	-4.42966	2.29317	2.44909
H	-6.05343	2.07482	0.59224
H	5.65167	2.76771	-0.13847
H	4.54009	4.93554	-0.48913
H	1.23349	-0.51122	-2.63898
H	2.31729	-0.38936	-4.02404
H	2.65782	0.53378	-2.55633
Al	-0.60678	-1.30147	0.00636
C	-0.63805	-2.45704	-1.62422
C	-1.18605	-2.28421	1.65326
H	-0.48897	-2.09743	2.48041
C	-2.62458	-2.36708	2.27291
H	-0.91235	-3.30070	1.31813
H	-0.20851	-1.88166	-2.45416
C	-1.79888	-3.31081	-2.19602
H	0.17471	-3.15575	-1.34802
C	-2.75628	-1.39630	3.46126
C	-2.85548	-3.79775	2.80548
C	-3.74178	-2.02064	1.26837
H	-3.62015	-1.00590	0.87041
H	-4.72678	-2.06375	1.75255
H	-3.76666	-2.71699	0.42611
H	-2.08649	-4.06615	3.54122
H	-2.81262	-4.53663	1.99576
H	-3.83591	-3.89152	3.29239
C	-1.34335	-3.96076	-3.52175
C	-3.03323	-2.43661	-2.48976
C	-2.16948	-4.44247	-1.22041
H	-1.07098	-3.19659	-4.26118
H	-2.13667	-4.58335	-3.95804
H	-0.46490	-4.59944	-3.36389
H	-1.30728	-5.09897	-1.04412
H	-2.98387	-5.06022	-1.62135

H	-2.48879	-4.05545	-0.25106
H	-5.22560	1.59009	-1.69028
H	-1.95634	-1.54899	4.19698
H	-3.71684	-1.53998	3.97361
H	-2.72164	-0.35906	3.12580
H	-3.36683	-1.88853	-1.60184
H	-3.87492	-3.04508	-2.84675
H	-2.80791	-1.69909	-3.26898

Compound **10**

C	2.21033	4.83267	0.59482
C	2.23215	3.40984	0.56327
C	1.05061	2.73661	0.30750
C	-0.13338	3.49976	0.09371
C	1.05682	5.56673	0.37434
C	-0.17563	4.90010	0.11011
C	-1.26743	2.67020	-0.14310
C	-2.48626	3.27712	-0.38999
C	-1.44578	5.49670	-0.14208
C	-2.55121	4.69917	-0.38588
C	0.64069	1.33338	0.19590
C	-0.76954	1.29064	-0.06724
N	-1.34092	0.08800	-0.22120
N	1.29707	0.16703	0.28903
C	-2.76428	0.00667	-0.33842
C	2.72618	0.17179	0.27557
C	-3.57766	0.27717	0.78312
C	-3.33916	-0.34970	-1.57241
C	-4.73270	-0.44232	-1.66171
C	-5.56360	-0.19332	-0.56647
C	-4.96404	0.17054	0.64396
C	3.41079	0.54572	-0.90204
C	3.43679	-0.20150	1.43202
C	4.83510	-0.21481	1.38475
C	4.80848	0.51399	-0.89907
C	5.54095	0.13061	0.22903
H	-3.51189	5.17098	-0.57883
H	-3.38235	2.69420	-0.57811
H	-1.54168	6.58043	-0.14268
H	1.08649	6.65395	0.40061
H	3.14127	5.35779	0.79562
H	3.16303	2.87688	0.73064
H	5.33896	0.79276	-1.80867
H	5.38591	-0.49675	2.28119
H	-5.17861	-0.71017	-2.61876
H	-5.59325	0.37187	1.51008
C	-7.06257	-0.34070	-0.67553
H	-7.40954	-0.17260	-1.70111
H	-7.58456	0.36485	-0.01917
H	-7.38035	-1.35134	-0.38449
C	-2.48014	-0.60697	-2.78608
H	-1.66662	0.12199	-2.86348
H	-3.07684	-0.55985	-3.70273
H	-2.01363	-1.59795	-2.74366
C	-2.97821	0.67867	2.10944
H	-2.10099	0.07082	2.35031
H	-3.70900	0.56494	2.91630
H	-2.65145	1.72597	2.09784
C	2.66708	0.98607	-2.14155
H	1.77704	0.37337	-2.31461
H	3.30960	0.91182	-3.02434

H	2.33409	2.02770	-2.05355
C	2.71233	-0.55382	2.70769
H	1.87307	0.12487	2.89213
H	3.39048	-0.51088	3.56600
H	2.29434	-1.56598	2.66431
C	7.04913	0.06543	0.18900
H	7.46619	0.81877	-0.48886
H	7.39054	-0.91653	-0.16630
H	7.48478	0.22200	1.18210
Al	0.03094	-1.33994	0.04154
C	0.39915	-2.38903	-1.61201
C	-0.32158	-2.30594	1.75627
H	-0.55339	-1.53300	2.50899
H	0.64790	-2.71536	2.08584
C	-1.36883	-3.44900	1.89914
H	-0.49136	-3.03948	-1.67769
C	1.67074	-3.28984	-1.78234
H	0.31294	-1.73838	-2.49529
C	2.33815	-3.62841	-0.43328
C	2.71619	-2.57218	-2.65631
C	1.27441	-4.60595	-2.48253
C	-2.74688	-3.02271	1.36384
C	-1.51718	-3.81449	3.39164
C	-0.91329	-4.70698	1.13695
H	3.07931	-1.66215	-2.17148
H	2.29827	-2.29928	-3.63383
H	3.58679	-3.21843	-2.83183
H	-1.87864	-2.95500	3.97092
H	-0.55338	-4.12179	3.81735
H	-2.22790	-4.63984	3.53689
H	0.56468	-5.17905	-1.87234
H	2.14953	-5.24470	-2.66539
H	0.79653	-4.40356	-3.44961
H	-3.12597	-2.14192	1.89128
H	-3.48351	-3.82737	1.49058
H	-2.71247	-2.77517	0.29539
H	0.04570	-5.07743	1.52045
H	-0.79319	-4.50785	0.06672
H	-1.64726	-5.51650	1.24516
H	2.69889	-2.72071	0.06936
H	3.20833	-4.28264	-0.57966
H	1.64768	-4.14192	0.24163

Compound **11**

C	3.81349	0.70450	0.24023
C	3.81854	-0.67669	-0.24235
C	2.58094	1.40437	0.39380
C	1.31871	0.71411	0.13738
C	1.32396	-0.70539	-0.13778
C	2.59127	-1.38620	-0.39421
C	5.02269	-1.32452	-0.58819
C	5.04765	-2.62826	-1.05590
C	2.64563	-2.71253	-0.89068
C	3.84408	-3.32664	-1.20928
C	2.62537	2.73054	0.89163
C	3.81933	3.35381	1.20930
C	5.02818	2.66515	1.05360
C	5.01294	1.36158	0.58496
H	5.96210	-0.78823	-0.51459
H	5.99515	-3.09420	-1.31502
H	3.84058	-4.34462	-1.59053
H	1.73385	-3.26982	-1.03337
H	5.95646	0.83278	0.50987
H	5.97232	3.13836	1.31183
H	3.80829	4.37133	1.59166
H	1.70933	3.28029	1.03636
N	0.09384	-1.27965	-0.21517
N	0.08446	1.27899	0.21535
C	-0.12025	-2.66238	0.10545
C	-0.14091	2.66080	-0.10129
C	-0.65341	3.54501	0.86914
C	-0.97945	4.85243	0.48474
C	-0.79198	5.28701	-0.82328
C	-0.24638	4.41462	-1.76473
C	0.09196	3.10143	-1.42730
C	-0.62516	-3.55377	-0.86246
C	0.11659	-3.09718	1.43260
C	-0.20904	-4.41275	1.77352
C	-0.74603	-5.29281	0.83438
C	-0.93820	-4.86331	-0.47471
C	-0.73221	-3.16690	-2.31799
H	-0.06613	-2.33357	-2.55758
H	-1.74782	-2.86772	-2.59490
H	-0.46143	-4.01533	-2.95672
C	0.70030	-2.17188	2.47282
H	0.18157	-1.20777	2.49158
H	1.75993	-1.96648	2.27647
H	0.62514	-2.61582	3.47021
C	-0.75403	3.15493	2.32435

H	-0.09590	2.31343	2.55649
H	-1.77120	2.86763	2.60838
H	-0.46800	3.99847	2.96309
C	0.68531	2.18468	-2.46960
H	0.60669	2.63059	-3.46584
H	0.17610	1.21557	-2.49145
H	1.74672	1.98906	-2.27283
H	-1.32054	-5.55424	-1.22381
H	-0.99745	-6.31133	1.11997
H	-0.04229	-4.74679	2.79555
H	-1.36800	5.53774	1.23582
H	-1.05347	6.30370	-1.10631
H	-0.08282	4.75296	-2.78587
Al	-1.40202	-0.00563	-0.00153
C	-2.56714	-0.87820	1.38334
C	-2.57047	0.85922	-1.38848
C	-3.27971	-0.18328	2.56721
C	-3.27395	0.16006	-2.57514
C	-3.97005	-1.13493	-2.11861
C	-4.34918	1.09965	-3.16430
C	-2.25618	0.11792	3.67713
C	-4.35370	-1.12818	3.15001
C	-3.97885	1.10942	2.10892
H	-3.90649	-2.07932	3.46530
H	-5.12488	-1.35414	2.40263
H	-4.85148	-0.68330	4.02300
H	-1.84947	-0.81557	4.08671
H	-2.70980	0.67684	4.50670
H	-1.41297	0.70027	3.29595
H	-2.06503	-1.77261	1.77568
H	-3.35159	-1.28218	0.71780
H	-5.12480	1.32336	-2.42086
H	-4.84096	0.65147	-4.03900
H	-3.90450	2.05224	-3.47879
H	-3.26361	-1.84806	-1.67893
H	-4.47608	-1.63558	-2.95505
H	-4.72596	-0.91840	-1.35299
H	-2.07344	1.75744	-1.77854
H	-3.35988	1.25718	-0.72529
C	-2.24352	-0.13771	-3.67961
H	-1.39885	-0.71467	-3.29336
H	-1.83991	0.79726	-4.08888
H	-2.69005	-0.70050	-4.51041
H	-4.49126	1.60669	2.94350
H	-4.73000	0.89096	1.33917
H	-3.27294	1.82606	1.67411

EPR Parameter

Compound **6**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.00317	-3.56005	-1.27032	-1.18751
2	C(13)	0.00275	3.08830	1.10198	1.03015
3	C(13)	0.00389	4.37488	1.56106	1.45930
4	H(1)	-0.00049	-2.17900	-0.77752	-0.72683
5	C(13)	-0.01331	-14.96739	-5.34074	-4.99258
6	C(13)	0.01219	13.69946	4.88831	4.56965
7	C(13)	-0.00633	-7.12071	-2.54085	-2.37521
8	C(13)	0.00362	4.06948	1.45209	1.35743
9	C(13)	-0.01281	-14.39674	-5.13712	-4.80224
10	C(13)	0.00239	2.68879	0.95943	0.89688
11	C(13)	-0.00296	-3.32229	-1.18548	-1.10820
12	C(13)	0.00740	8.31994	2.96876	2.77523
13	C(13)	0.00890	10.00218	3.56903	3.33637
14	N(14)	0.04281	13.83236	4.93573	4.61398
15	N(14)	0.04348	14.04958	5.01324	4.68643
16	H(1)	-0.00055	-2.45960	-0.87765	-0.82043
17	H(1)	0.00010	0.43005	0.15345	0.14345
18	H(1)	-0.00045	-2.02973	-0.72426	-0.67704
19	C(13)	-0.01004	-11.29034	-4.02867	-3.76605
20	C(13)	-0.01029	-11.56483	-4.12662	-3.85761
21	C(13)	0.01186	13.32769	4.75565	4.44564
22	C(13)	0.01258	14.14035	5.04563	4.71671
23	C(13)	0.00043	0.48736	0.17390	0.16256
24	C(13)	0.00033	0.37226	0.13283	0.12417
25	C(13)	0.00075	0.84579	0.30180	0.28212
26	C(13)	0.01243	13.97031	4.98495	4.65999
27	C(13)	0.01295	14.55394	5.19321	4.85467
28	C(13)	0.00104	1.17193	0.41817	0.39091
29	C(13)	0.00005	0.05519	0.01969	0.01841
30	C(13)	0.00099	1.11632	0.39833	0.37236
31	H(1)	-0.00001	-0.04454	-0.01589	-0.01486
32	H(1)	0.00024	1.07712	0.38434	0.35929
33	H(1)	0.00022	0.96970	0.34601	0.32346
34	C(13)	0.00050	0.55753	0.19894	0.18597
35	C(13)	-0.00003	-0.03448	-0.01230	-0.01150
36	H(1)	0.00002	0.09234	0.03295	0.03080
37	H(1)	0.00001	0.04376	0.01561	0.01460
38	H(1)	-0.00001	-0.04007	-0.01430	-0.01337
39	C(13)	0.00034	0.38113	0.13600	0.12713
40	H(1)	0.00000	0.01996	0.00712	0.00666
41	H(1)	0.00002	0.09448	0.03371	0.03151

42	H(1)	0.00013	0.57617	0.20559	0.19219
43	H(1)	-0.00002	-0.08901	-0.03176	-0.02969
44	C(13)	0.00005	0.05184	0.01850	0.01729
45	C(13)	0.00027	0.29871	0.10659	0.09964
46	C(13)	0.00016	0.17560	0.06266	0.05857
47	H(1)	0.00000	0.02070	0.00739	0.00690
48	H(1)	-0.00003	-0.14157	-0.05052	-0.04722
49	H(1)	-0.00000	-0.01916	-0.00684	-0.00639
50	H(1)	-0.00001	-0.05076	-0.01811	-0.01693
51	C(13)	-0.00038	-0.43242	-0.15430	-0.14424
52	C(13)	0.00179	2.00857	0.71671	0.66999
53	H(1)	0.00012	0.51813	0.18488	0.17283
54	C(13)	0.00120	1.34582	0.48022	0.44892
55	C(13)	0.00125	1.41003	0.50313	0.47034
56	C(13)	0.00053	0.59283	0.21154	0.19775
57	C(13)	-0.00003	-0.03245	-0.01158	-0.01082
58	H(1)	0.00014	0.60610	0.21627	0.20217
59	H(1)	0.00007	0.33345	0.11898	0.11123
60	H(1)	-0.00000	-0.01005	-0.00359	-0.00335
61	H(1)	0.00002	0.10450	0.03729	0.03486
62	H(1)	0.00011	0.49458	0.17648	0.16497
63	H(1)	0.00000	0.01021	0.00364	0.00341
64	H(1)	0.00003	0.14135	0.05044	0.04715
65	H(1)	-0.00002	-0.10501	-0.03747	-0.03503
66	H(1)	0.00002	0.07899	0.02819	0.02635
67	H(1)	-0.00001	-0.03803	-0.01357	-0.01269
68	H(1)	0.00013	0.58758	0.20966	0.19599
69	H(1)	-0.00012	-0.55244	-0.19713	-0.18428
70	H(1)	-0.00037	-1.64487	-0.58693	-0.54867
71	H(1)	0.00026	1.15416	0.41183	0.38498
72	H(1)	-0.00005	-0.21403	-0.07637	-0.07139
73	H(1)	0.00010	0.46192	0.16483	0.15408
74	H(1)	-0.00059	-2.62584	-0.93696	-0.87589
75	H(1)	-0.00005	-0.20959	-0.07479	-0.06991
76	H(1)	-0.00012	-0.55828	-0.19921	-0.18622
77	H(1)	0.00012	0.55269	0.19721	0.18436
78	Al(27)	-0.01778	-20.72198	-7.39412	-6.91211
79	C(13)	0.01061	11.92566	4.25537	3.97797
80	C(13)	0.01173	13.18732	4.70556	4.39882
81	H(1)	-0.00029	-1.31693	-0.46991	-0.43928
82	C(13)	-0.00019	-0.21492	-0.07669	-0.07169
83	H(1)	0.00008	0.34568	0.12335	0.11531
84	H(1)	-0.00018	-0.79262	-0.28283	-0.26439
85	C(13)	0.00026	0.28834	0.10289	0.09618
86	H(1)	-0.00027	-1.20953	-0.43159	-0.40346
87	H(1)	-0.00001	-0.04119	-0.01470	-0.01374

88	C(13)	0.00068	0.76411	0.27265	0.25488
89	C(13)	0.00005	0.05644	0.02014	0.01883
90	H(1)	-0.00002	-0.08492	-0.03030	-0.02833
91	H(1)	-0.00001	-0.05438	-0.01941	-0.01814
92	H(1)	-0.00000	-0.01749	-0.00624	-0.00583
93	H(1)	-0.00000	-0.00578	-0.00206	-0.00193
94	H(1)	0.00000	0.00680	0.00243	0.00227
95	H(1)	0.00011	0.51243	0.18285	0.17093
96	C(13)	0.00070	0.78695	0.28080	0.26250
97	H(1)	-0.00002	-0.07947	-0.02836	-0.02651
98	C(13)	0.00013	0.15069	0.05377	0.05027
99	H(1)	0.00001	0.02918	0.01041	0.00973
100	H(1)	0.00012	0.51624	0.18421	0.17220
101	H(1)	-0.00000	-0.02078	-0.00741	-0.00693
102	H(1)	-0.00005	-0.20248	-0.07225	-0.06754
103	H(1)	-0.00006	-0.28928	-0.10322	-0.09649
104	H(1)	-0.00004	-0.18822	-0.06716	-0.06278
105	H(1)	0.00026	1.14016	0.40684	0.38032

Compound **7**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.00324	-3.64622	-1.30106	-1.21625
2	C(13)	0.00282	3.17088	1.13145	1.05769
3	C(13)	-0.01318	-14.81536	-5.28649	-4.94187
4	C(13)	0.01281	14.40341	5.13950	4.80446
5	C(13)	0.00391	4.40004	1.57004	1.46769
6	C(13)	-0.00661	-7.43412	-2.65268	-2.47975
7	C(13)	-0.01318	-14.81575	-5.28663	-4.94200
8	C(13)	0.00282	3.17139	1.13163	1.05786
9	C(13)	0.00391	4.40051	1.57021	1.46785
10	C(13)	-0.00324	-3.64660	-1.30120	-1.21638
11	C(13)	0.00888	9.98662	3.56347	3.33118
12	C(13)	0.00888	9.98822	3.56405	3.33171
13	N(14)	0.04388	14.17883	5.05936	4.72955
14	N(14)	0.04388	14.17828	5.05916	4.72936
15	C(13)	-0.00987	-11.09839	-3.96018	-3.70202
16	C(13)	-0.00987	-11.09899	-3.96040	-3.70223
17	C(13)	0.01303	14.65086	5.22779	4.88700
18	C(13)	0.01225	13.76676	4.91232	4.59210
19	C(13)	0.00078	0.87766	0.31317	0.29275
20	C(13)	0.00016	0.18367	0.06554	0.06126
21	C(13)	0.00111	1.24408	0.44392	0.41498
22	C(13)	0.01303	14.65007	5.22751	4.88674
23	C(13)	0.01225	13.76682	4.91234	4.59212
24	C(13)	0.00078	0.87721	0.31301	0.29261
25	C(13)	0.00111	1.24326	0.44362	0.41471
26	C(13)	0.00016	0.18438	0.06579	0.06150
27	H(1)	0.00011	0.50028	0.17851	0.16688
28	H(1)	-0.00048	-2.16752	-0.77343	-0.72301
29	H(1)	-0.00059	-2.62833	-0.93785	-0.87672
30	H(1)	-0.00059	-2.62805	-0.93775	-0.87662
31	H(1)	0.00011	0.50023	0.17850	0.16686
32	H(1)	-0.00048	-2.16732	-0.77335	-0.72294
33	H(1)	0.00026	1.18166	0.42165	0.39416
34	H(1)	0.00024	1.06286	0.37925	0.35453
35	H(1)	0.00024	1.06273	0.37921	0.35449
36	H(1)	0.00026	1.18168	0.42165	0.39416
37	C(13)	-0.00007	-0.07539	-0.02690	-0.02515
38	H(1)	-0.00000	-0.00121	-0.00043	-0.00040
39	H(1)	0.00003	0.12640	0.04510	0.04216
40	H(1)	0.00003	0.15226	0.05433	0.05079
41	C(13)	0.00011	0.12065	0.04305	0.04024
42	H(1)	0.00007	0.29227	0.10429	0.09749
43	H(1)	0.00011	0.47028	0.16781	0.15687
44	H(1)	0.00031	1.38912	0.49567	0.46336
45	C(13)	-0.00026	-0.29517	-0.10533	-0.09846
46	H(1)	0.00003	0.12068	0.04306	0.04025
47	H(1)	-0.00006	-0.25167	-0.08980	-0.08395
48	H(1)	-0.00006	-0.24717	-0.08820	-0.08245
49	C(13)	-0.00026	-0.29547	-0.10543	-0.09856

50	H(1)	0.00003	0.12041	0.04297	0.04017
51	H(1)	-0.00006	-0.25186	-0.08987	-0.08401
52	H(1)	-0.00006	-0.24700	-0.08813	-0.08239
53	C(13)	0.00011	0.12035	0.04294	0.04014
54	H(1)	0.00007	0.29285	0.10450	0.09768
55	H(1)	0.00011	0.47072	0.16797	0.15702
56	H(1)	0.00031	1.38980	0.49592	0.46359
57	C(13)	-0.00007	-0.07557	-0.02697	-0.02521
58	H(1)	0.00003	0.12664	0.04519	0.04224
59	H(1)	0.00003	0.15288	0.05455	0.05099
60	H(1)	-0.00000	-0.00115	-0.00041	-0.00038
61	Al(27)	-0.01817	-21.17520	-7.55584	-7.06328
62	C(13)	0.01221	13.72973	4.89911	4.57974
63	C(13)	0.01221	13.72711	4.89817	4.57887
64	H(1)	-0.00025	-1.11937	-0.39942	-0.37338
65	H(1)	-0.00005	-0.23557	-0.08406	-0.07858
66	C(13)	0.00017	0.19411	0.06926	0.06475
67	H(1)	-0.00005	-0.23547	-0.08402	-0.07854
68	C(13)	0.00017	0.19416	0.06928	0.06477
69	H(1)	-0.00025	-1.11933	-0.39940	-0.37337
70	H(1)	0.00000	0.02063	0.00736	0.00688
71	C(13)	-0.00003	-0.03814	-0.01361	-0.01272
72	C(13)	0.00096	1.07448	0.38340	0.35841
73	C(13)	-0.00003	-0.03807	-0.01358	-0.01270
74	C(13)	0.00096	1.07438	0.38337	0.35838
75	H(1)	0.00000	0.02065	0.00737	0.00689
76	H(1)	-0.00002	-0.06874	-0.02453	-0.02293
77	H(1)	-0.00001	-0.03633	-0.01296	-0.01212
78	H(1)	-0.00002	-0.10971	-0.03915	-0.03660
79	H(1)	-0.00001	-0.02545	-0.00908	-0.00849
80	H(1)	0.00000	0.02191	0.00782	0.00731
81	H(1)	0.00012	0.54506	0.19449	0.18181
82	H(1)	0.00000	0.02193	0.00783	0.00732
83	H(1)	0.00012	0.54514	0.19452	0.18184
84	H(1)	-0.00001	-0.02545	-0.00908	-0.00849
85	H(1)	-0.00001	-0.03631	-0.01296	-0.01211
86	H(1)	-0.00002	-0.10972	-0.03915	-0.03660
87	H(1)	-0.00002	-0.06876	-0.02453	-0.02294

Compound **8**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.00523	5.88259	2.09905	1.96222
2	C(13)	0.00386	4.33894	1.54824	1.44732
3	C(13)	-0.01201	-13.49901	-4.81678	-4.50279
4	C(13)	0.01068	12.01110	4.28586	4.00647
5	C(13)	0.00407	4.57528	1.63257	1.52615
6	C(13)	-0.00884	-9.93454	-3.54489	-3.31381
7	C(13)	-0.00464	-5.21789	-1.86187	-1.74050
8	C(13)	0.00590	6.62841	2.36518	2.21100
9	C(13)	0.00545	6.12945	2.18714	2.04456
10	C(13)	-0.00431	-4.84113	-1.72744	-1.61483
11	C(13)	0.00621	6.97790	2.48989	2.32758
12	C(13)	-0.00532	-5.98352	-2.13507	-1.99589
13	C(13)	0.00693	7.78864	2.77918	2.59801
14	C(13)	-0.00564	-6.34309	-2.26337	-2.11583
15	H(1)	0.00017	0.75775	0.27038	0.25276
16	H(1)	-0.00082	-3.64622	-1.30106	-1.21625
17	H(1)	0.00017	0.73892	0.26367	0.24648
18	H(1)	-0.00079	-3.55184	-1.26738	-1.18477
19	H(1)	0.00022	0.98642	0.35198	0.32903
20	H(1)	-0.00094	-4.18931	-1.49485	-1.39740
21	H(1)	0.00025	1.13428	0.40474	0.37836
22	H(1)	-0.00094	-4.19351	-1.49635	-1.39881
23	N(14)	0.04958	16.01904	5.71599	5.34338
24	N(14)	0.04440	14.34687	5.11932	4.78560
25	C(13)	-0.00837	-9.41463	-3.35938	-3.14038
26	C(13)	-0.00654	-7.35004	-2.62268	-2.45171
27	C(13)	0.00746	8.38630	2.99244	2.79737
28	C(13)	-0.00115	-1.29040	-0.46045	-0.43043
29	C(13)	0.00141	1.58527	0.56566	0.52879
30	C(13)	0.00078	0.87133	0.31091	0.29065
31	C(13)	0.01349	15.16808	5.41235	5.05953
32	C(13)	0.01550	17.42014	6.21594	5.81073
33	C(13)	0.01039	11.68170	4.16832	3.89659
34	C(13)	0.00042	0.47042	0.16786	0.15692
35	C(13)	-0.00001	-0.01578	-0.00563	-0.00526
36	C(13)	0.00176	1.97977	0.70643	0.66038
37	C(13)	-0.00023	-0.25701	-0.09171	-0.08573
38	H(1)	0.00002	0.08452	0.03016	0.02819
39	H(1)	-0.00012	-0.55179	-0.19689	-0.18406
40	H(1)	-0.00011	-0.49027	-0.17494	-0.16353
41	C(13)	0.00034	0.37760	0.13474	0.12595
42	H(1)	0.00018	0.78593	0.28044	0.26216
43	H(1)	0.00008	0.35076	0.12516	0.11700

44	H(1)	0.00010	0.46922	0.16743	0.15651
45	C(13)	0.00044	0.49415	0.17633	0.16483
46	H(1)	0.00010	0.45796	0.16341	0.15276
47	H(1)	0.00050	2.24114	0.79969	0.74756
48	H(1)	0.00031	1.37402	0.49028	0.45832
49	C(13)	-0.00066	-0.73856	-0.26354	-0.24636
50	H(1)	0.00009	0.40043	0.14288	0.13357
51	H(1)	0.00048	2.13013	0.76008	0.71053
52	H(1)	0.00006	0.28830	0.10287	0.09617
53	H(1)	0.00037	1.63349	0.58287	0.54487
54	H(1)	-0.00000	-0.01796	-0.00641	-0.00599
55	H(1)	0.00018	0.80990	0.28899	0.27015
56	H(1)	0.00013	0.59233	0.21136	0.19758
57	H(1)	-0.00019	-0.85355	-0.30457	-0.28471
58	H(1)	0.00036	1.61823	0.57742	0.53978
59	Al(27)	-0.01887	-21.99053	-7.84677	-7.33525
60	C(13)	0.01578	17.73634	6.32877	5.91621
61	C(13)	0.00862	9.69086	3.45794	3.23252
62	C(13)	-0.00074	-0.83440	-0.29773	-0.27832
63	C(13)	-0.00026	-0.29706	-0.10600	-0.09909
64	C(13)	-0.00002	-0.02210	-0.00788	-0.00737
65	C(13)	0.00067	0.75850	0.27065	0.25301
66	C(13)	0.00040	0.45525	0.16245	0.15186
67	C(13)	0.00062	0.69987	0.24973	0.23345
68	H(1)	-0.00000	-0.00552	-0.00197	-0.00184
69	H(1)	-0.00001	-0.03659	-0.01306	-0.01221
70	H(1)	0.00004	0.16726	0.05968	0.05579
71	H(1)	0.00011	0.48394	0.17268	0.16143
72	H(1)	0.00003	0.13565	0.04840	0.04525
73	H(1)	-0.00001	-0.06101	-0.02177	-0.02035
74	H(1)	-0.00001	-0.03402	-0.01214	-0.01135
75	H(1)	-0.00025	-1.10254	-0.39342	-0.36777
76	H(1)	0.00024	1.05101	0.37503	0.35058
77	H(1)	-0.00000	-0.01375	-0.00491	-0.00459
78	H(1)	0.00008	0.35394	0.12630	0.11806
79	H(1)	-0.00000	-0.01248	-0.00445	-0.00416
80	H(1)	-0.00001	-0.05120	-0.01827	-0.01708
81	H(1)	-0.00001	-0.04907	-0.01751	-0.01637
82	H(1)	-0.00000	-0.00187	-0.00067	-0.00063
83	H(1)	-0.00025	-1.12377	-0.40099	-0.37485
84	H(1)	0.00035	1.56683	0.55908	0.52264
85	H(1)	0.00004	0.17091	0.06099	0.05701

Compound **9**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.00267	-2.99965	-1.07035	-1.00057
2	C(13)	0.00200	2.24999	0.80285	0.75051
3	C(13)	0.00330	3.70820	1.32318	1.23692
4	H(1)	-0.00039	-1.75904	-0.62767	-0.58675
5	C(13)	-0.01227	-13.78858	-4.92011	-4.59937
6	C(13)	0.01228	13.79999	4.92418	4.60318
7	C(13)	-0.00633	-7.11457	-2.53865	-2.37316
8	C(13)	0.00419	4.70884	1.68023	1.57070
9	C(13)	-0.01376	-15.46436	-5.51807	-5.15836
10	C(13)	0.00310	3.48083	1.24205	1.16108
11	C(13)	-0.00341	-3.83312	-1.36775	-1.27859
12	C(13)	0.01029	11.56752	4.12758	3.85851
13	C(13)	0.00577	6.48342	2.31344	2.16263
14	N(14)	0.04196	13.55765	4.83771	4.52234
15	N(14)	0.04622	14.93352	5.32865	4.98129
16	H(1)	-0.00063	-2.82864	-1.00933	-0.94353
17	H(1)	0.00011	0.49428	0.17637	0.16487
18	H(1)	-0.00054	-2.43262	-0.86802	-0.81143
19	C(13)	-0.01010	-11.35135	-4.05044	-3.78640
20	C(13)	-0.00920	-10.33898	-3.68920	-3.44871
21	C(13)	0.01059	11.90717	4.24878	3.97181
22	C(13)	0.01376	15.47124	5.52052	5.16065
23	C(13)	0.00115	1.29325	0.46146	0.43138
24	C(13)	0.00005	0.06178	0.02204	0.02061
25	C(13)	0.00066	0.74269	0.26501	0.24774
26	C(13)	0.01309	14.71797	5.25174	4.90939
27	C(13)	0.01215	13.66343	4.87545	4.55763
28	C(13)	0.00117	1.30973	0.46734	0.43688
29	C(13)	0.00007	0.08379	0.02990	0.02795
30	C(13)	0.00070	0.79144	0.28241	0.26400
31	H(1)	-0.00001	-0.06144	-0.02192	-0.02049
32	H(1)	0.00027	1.22575	0.43738	0.40887
33	H(1)	0.00020	0.87334	0.31163	0.29132
34	C(13)	0.00069	0.78046	0.27849	0.26033
35	C(13)	-0.00007	-0.08114	-0.02895	-0.02706
36	H(1)	0.00004	0.18813	0.06713	0.06275
37	H(1)	0.00002	0.07925	0.02828	0.02643
38	H(1)	0.00000	0.00572	0.00204	0.00191
39	C(13)	0.00036	0.40793	0.14556	0.13607
40	H(1)	-0.00000	-0.00921	-0.00329	-0.00307
41	H(1)	0.00003	0.13028	0.04649	0.04346
42	H(1)	0.00013	0.57150	0.20393	0.19063
43	H(1)	-0.00003	-0.12279	-0.04381	-0.04096

44	C(13)	-0.00016	-0.17906	-0.06389	-0.05973
45	C(13)	-0.00033	-0.37385	-0.13340	-0.12470
46	C(13)	0.00011	0.12170	0.04343	0.04059
47	H(1)	-0.00003	-0.13138	-0.04688	-0.04382
48	H(1)	-0.00004	-0.16028	-0.05719	-0.05346
49	H(1)	-0.00002	-0.09021	-0.03219	-0.03009
50	H(1)	-0.00001	-0.04689	-0.01673	-0.01564
51	C(13)	-0.00051	-0.57104	-0.20376	-0.19048
52	C(13)	0.00300	3.37684	1.20494	1.12639
53	H(1)	0.00007	0.31630	0.11287	0.10551
54	C(13)	0.00100	1.12098	0.39999	0.37392
55	C(13)	-0.00016	-0.18212	-0.06499	-0.06075
56	C(13)	0.00006	0.06592	0.02352	0.02199
57	C(13)	0.00005	0.05338	0.01905	0.01781
58	H(1)	0.00000	0.01472	0.00525	0.00491
59	H(1)	-0.00001	-0.04486	-0.01601	-0.01496
60	H(1)	-0.00001	-0.03180	-0.01135	-0.01061
61	H(1)	-0.00001	-0.04678	-0.01669	-0.01561
62	H(1)	-0.00026	-1.15226	-0.41115	-0.38435
63	H(1)	0.00013	0.57468	0.20506	0.19169
64	H(1)	0.00020	0.90975	0.32462	0.30346
65	H(1)	-0.00003	-0.13590	-0.04849	-0.04533
66	H(1)	0.00000	0.00313	0.00112	0.00105
67	H(1)	-0.00001	-0.03444	-0.01229	-0.01149
68	H(1)	0.00003	0.11334	0.04044	0.03781
69	H(1)	-0.00019	-0.84387	-0.30111	-0.28148
70	H(1)	-0.00052	-2.32157	-0.82840	-0.77439
71	H(1)	0.00031	1.38820	0.49534	0.46305
72	H(1)	-0.00002	-0.08035	-0.02867	-0.02680
73	H(1)	0.00009	0.38382	0.13696	0.12803
74	H(1)	-0.00051	-2.26340	-0.80764	-0.75499
75	H(1)	-0.00007	-0.32269	-0.11514	-0.10764
76	H(1)	-0.00013	-0.57167	-0.20399	-0.19069
77	H(1)	0.00007	0.29470	0.10516	0.09830
78	Al(27)	-0.01704	-19.86413	-7.08802	-6.62596
79	C(13)	0.01101	12.37500	4.41571	4.12785
80	C(13)	0.00921	10.35758	3.69584	3.45492
81	H(1)	-0.00024	-1.08053	-0.38556	-0.36043
82	C(13)	0.00018	0.20673	0.07376	0.06896
83	H(1)	-0.00004	-0.17858	-0.06372	-0.05957
84	H(1)	-0.00022	-1.00098	-0.35717	-0.33389
85	C(13)	0.00080	0.89597	0.31970	0.29886
86	H(1)	-0.00028	-1.23205	-0.43962	-0.41097
87	C(13)	-0.00001	-0.01339	-0.00478	-0.00447
88	C(13)	0.00051	0.57462	0.20504	0.19167
89	C(13)	0.00012	0.13188	0.04706	0.04399

90	H(1)	-0.00007	-0.31013	-0.11066	-0.10345
91	H(1)	-0.00004	-0.17170	-0.06127	-0.05727
92	H(1)	-0.00000	-0.02199	-0.00785	-0.00733
93	H(1)	0.00000	0.02084	0.00744	0.00695
94	H(1)	0.00001	0.04280	0.01527	0.01428
95	H(1)	0.00011	0.48546	0.17322	0.16193
96	C(13)	0.00055	0.62085	0.22153	0.20709
97	C(13)	-0.00005	-0.05160	-0.01841	-0.01721
98	C(13)	-0.00006	-0.07054	-0.02517	-0.02353
99	H(1)	-0.00000	-0.01496	-0.00534	-0.00499
100	H(1)	0.00010	0.46158	0.16470	0.15397
101	H(1)	0.00000	0.00016	0.00006	0.00005
102	H(1)	-0.00000	-0.00272	-0.00097	-0.00091
103	H(1)	0.00000	0.01232	0.00440	0.00411
104	H(1)	-0.00000	-0.01571	-0.00561	-0.00524
105	H(1)	0.00022	0.98243	0.35055	0.32770
106	H(1)	-0.00000	-0.00937	-0.00334	-0.00313
107	H(1)	-0.00000	-0.00907	-0.00324	-0.00302
108	H(1)	-0.00001	-0.03886	-0.01387	-0.01296
109	H(1)	-0.00009	-0.38511	-0.13742	-0.12846
110	H(1)	-0.00006	-0.28645	-0.10221	-0.09555
111	H(1)	-0.00001	-0.03599	-0.01284	-0.01200

Compound **10**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	-0.00322	-3.61507	-1.28995	-1.20586
2	C(13)	0.00291	3.26672	1.16565	1.08966
3	C(13)	-0.01319	-14.82964	-5.29158	-4.94664
4	C(13)	0.01243	13.97446	4.98644	4.66138
5	C(13)	0.00395	4.43726	1.58332	1.48011
6	C(13)	-0.00640	-7.19207	-2.56631	-2.39902
7	C(13)	-0.01256	-14.12300	-5.03944	-4.71092
8	C(13)	0.00238	2.67086	0.95303	0.89090
9	C(13)	0.00354	3.98459	1.42180	1.32912
10	C(13)	-0.00290	-3.26336	-1.16445	-1.08854
11	C(13)	0.00971	10.91273	3.89393	3.64010
12	C(13)	0.00755	8.48602	3.02802	2.83063
13	N(14)	0.04437	14.33683	5.11574	4.78225
14	N(14)	0.04494	14.52168	5.18170	4.84391
15	C(13)	-0.01038	-11.67014	-4.16420	-3.89274
16	C(13)	-0.00961	-10.80753	-3.85640	-3.60500
17	C(13)	0.01276	14.34279	5.11786	4.78424
18	C(13)	0.01173	13.19084	4.70682	4.39999
19	C(13)	-0.00013	-0.14679	-0.05238	-0.04896
20	C(13)	0.00101	1.13572	0.40525	0.37883
21	C(13)	0.00043	0.47830	0.17067	0.15954
22	C(13)	0.01307	14.68815	5.24110	4.89944
23	C(13)	0.01084	12.18400	4.34755	4.06414
24	C(13)	-0.00039	-0.44232	-0.15783	-0.14754
25	C(13)	0.00054	0.60304	0.21518	0.20115
26	C(13)	0.00109	1.22115	0.43574	0.40733
27	H(1)	0.00010	0.43029	0.15354	0.14353
28	H(1)	-0.00044	-1.95814	-0.69871	-0.65316
29	H(1)	-0.00054	-2.41046	-0.86011	-0.80404
30	H(1)	-0.00059	-2.65072	-0.94584	-0.88418
31	H(1)	0.00011	0.47720	0.17028	0.15918
32	H(1)	-0.00050	-2.25354	-0.80412	-0.75170
33	H(1)	0.00031	1.40747	0.50222	0.46948
34	H(1)	0.00022	0.97282	0.34713	0.32450
35	H(1)	0.00024	1.08766	0.38810	0.36280
36	H(1)	0.00029	1.30756	0.46657	0.43616
37	C(13)	-0.00029	-0.32989	-0.11771	-0.11004
38	H(1)	0.00002	0.11060	0.03946	0.03689
39	H(1)	0.00010	0.43865	0.15652	0.14632
40	H(1)	0.00022	0.97944	0.34949	0.32671
41	C(13)	0.00039	0.44234	0.15784	0.14755
42	H(1)	0.00015	0.66351	0.23676	0.22132
43	H(1)	0.00026	1.15144	0.41086	0.38408

44	H(1)	0.00047	2.09720	0.74833	0.69955
45	C(13)	-0.00068	-0.76270	-0.27215	-0.25441
46	H(1)	0.00008	0.35115	0.12530	0.11713
47	H(1)	-0.00010	-0.42683	-0.15230	-0.14238
48	H(1)	-0.00000	-0.01896	-0.00677	-0.00632
49	C(13)	-0.00075	-0.83993	-0.29971	-0.28017
50	H(1)	0.00013	0.57500	0.20518	0.19180
51	H(1)	-0.00008	-0.37395	-0.13344	-0.12474
52	H(1)	0.00002	0.09766	0.03485	0.03258
53	C(13)	0.00039	0.43595	0.15556	0.14542
54	H(1)	0.00013	0.57912	0.20664	0.19317
55	H(1)	0.00026	1.16138	0.41441	0.38739
56	H(1)	0.00049	2.17916	0.77758	0.72689
57	C(13)	-0.00031	-0.35122	-0.12532	-0.11715
58	H(1)	0.00010	0.44467	0.15867	0.14833
59	H(1)	0.00024	1.06608	0.38040	0.35561
60	H(1)	0.00003	0.13187	0.04706	0.04399
61	Al(27)	-0.01759	-20.50579	-7.31698	-6.84000
62	C(13)	0.01174	13.19599	4.70866	4.40171
63	C(13)	0.01224	13.76527	4.91179	4.59160
64	H(1)	-0.00018	-0.78289	-0.27935	-0.26114
65	H(1)	-0.00000	-0.00282	-0.00101	-0.00094
66	C(13)	0.00030	0.33556	0.11974	0.11193
67	H(1)	0.00011	0.46940	0.16749	0.15657
68	C(13)	0.00005	0.05744	0.02050	0.01916
69	H(1)	-0.00021	-0.91821	-0.32764	-0.30628
70	C(13)	0.00012	0.13132	0.04686	0.04380
71	C(13)	0.00001	0.01104	0.00394	0.00368
72	C(13)	0.00061	0.68470	0.24432	0.22839
73	C(13)	0.00005	0.05574	0.01989	0.01859
74	C(13)	0.00067	0.75056	0.26782	0.25036
75	C(13)	-0.00004	-0.04541	-0.01620	-0.01515
76	H(1)	-0.00001	-0.03626	-0.01294	-0.01209
77	H(1)	-0.00000	-0.00103	-0.00037	-0.00034
78	H(1)	0.00001	0.06432	0.02295	0.02145
79	H(1)	-0.00000	-0.01819	-0.00649	-0.00607
80	H(1)	0.00001	0.03141	0.01121	0.01048
81	H(1)	0.00011	0.50726	0.18100	0.16920
82	H(1)	0.00001	0.05282	0.01885	0.01762
83	H(1)	0.00012	0.55476	0.19795	0.18505
84	H(1)	0.00001	0.03162	0.01128	0.01055
85	H(1)	-0.00002	-0.09720	-0.03468	-0.03242
86	H(1)	-0.00004	-0.19522	-0.06966	-0.06512
87	H(1)	-0.00003	-0.11926	-0.04256	-0.03978
88	H(1)	0.00000	0.01825	0.00651	0.00609
89	H(1)	-0.00000	-0.01558	-0.00556	-0.00520

90	H(1)	0.00001	0.04104	0.01464	0.01369
91	H(1)	-0.00004	-0.16287	-0.05811	-0.05433
92	H(1)	-0.00002	-0.09977	-0.03560	-0.03328
93	H(1)	-0.00000	-0.01244	-0.00444	-0.00415

Compound **11**

Isotropic Fermi Contact Couplings

	Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1	C(13)	0.00443	4.98349	1.77823	1.66231
2	C(13)	0.00446	5.01869	1.79079	1.67405
3	C(13)	-0.01177	-13.23729	-4.72339	-4.41548
4	C(13)	0.00878	9.87544	3.52380	3.29409
5	C(13)	0.00890	10.00337	3.56945	3.33677
6	C(13)	-0.01181	-13.27646	-4.73737	-4.42855
7	C(13)	-0.00498	-5.59979	-1.99814	-1.86789
8	C(13)	0.00645	7.24751	2.58609	2.41751
9	C(13)	0.00536	6.02838	2.15107	2.01085
10	C(13)	-0.00498	-5.59747	-1.99732	-1.86712
11	C(13)	0.00535	6.01053	2.14471	2.00490
12	C(13)	-0.00496	-5.57821	-1.99044	-1.86069
13	C(13)	0.00643	7.22732	2.57889	2.41077
14	C(13)	-0.00496	-5.58134	-1.99156	-1.86173
15	H(1)	0.00020	0.88297	0.31506	0.29453
16	H(1)	-0.00088	-3.92788	-1.40156	-1.31020
17	H(1)	0.00019	0.82985	0.29611	0.27681
18	H(1)	-0.00089	-3.99618	-1.42594	-1.33298
19	H(1)	0.00020	0.87879	0.31358	0.29313
20	H(1)	-0.00088	-3.91778	-1.39796	-1.30683
21	H(1)	0.00018	0.82488	0.29434	0.27515
22	H(1)	-0.00089	-3.98428	-1.42169	-1.32901
23	N(14)	0.04307	13.91756	4.96613	4.64240
24	N(14)	0.04309	13.92252	4.96790	4.64405
25	C(13)	-0.00763	-8.58159	-3.06212	-2.86251
26	C(13)	-0.00770	-8.65740	-3.08918	-2.88780
27	C(13)	0.00805	9.05091	3.22959	3.01906
28	C(13)	-0.00076	-0.85452	-0.30491	-0.28504
29	C(13)	0.00089	0.99947	0.35664	0.33339
30	C(13)	0.00111	1.25127	0.44649	0.41738
31	C(13)	0.01329	14.93694	5.32987	4.98243
32	C(13)	0.00804	9.03351	3.22338	3.01325
33	C(13)	0.01326	14.91017	5.32032	4.97350
34	C(13)	0.00111	1.25321	0.44718	0.41802
35	C(13)	0.00089	1.00154	0.35738	0.33408
36	C(13)	-0.00076	-0.85397	-0.30472	-0.28485
37	C(13)	0.00096	1.07461	0.38345	0.35845
38	H(1)	0.00010	0.42876	0.15299	0.14302
39	H(1)	0.00020	0.88834	0.31698	0.29632
40	H(1)	0.00028	1.25693	0.44850	0.41927
41	C(13)	-0.00032	-0.35475	-0.12658	-0.11833
42	H(1)	0.00014	0.61399	0.21909	0.20480
43	H(1)	0.00003	0.14246	0.05084	0.04752

44	H(1)	0.00001	0.04051	0.01446	0.01351
45	C(13)	0.00098	1.09796	0.39178	0.36624
46	H(1)	0.00009	0.41509	0.14811	0.13846
47	H(1)	0.00019	0.84406	0.30118	0.28155
48	H(1)	0.00028	1.26040	0.44974	0.42043
49	C(13)	-0.00033	-0.36559	-0.13045	-0.12195
50	H(1)	0.00001	0.03822	0.01364	0.01275
51	H(1)	0.00014	0.61903	0.22089	0.20649
52	H(1)	0.00003	0.14114	0.05036	0.04708
53	H(1)	0.00016	0.73649	0.26280	0.24567
54	H(1)	-0.00012	-0.53388	-0.19050	-0.17808
55	H(1)	0.00035	1.54286	0.55053	0.51464
56	H(1)	0.00017	0.74186	0.26471	0.24746
57	H(1)	-0.00012	-0.53206	-0.18985	-0.17748
58	H(1)	0.00034	1.54068	0.54975	0.51392
59	Al(27)	-0.02221	-25.88428	-9.23615	-8.63407
60	C(13)	0.01210	13.59927	4.85256	4.53623
61	C(13)	0.01214	13.65298	4.87172	4.55414
62	C(13)	-0.00064	-0.71878	-0.25648	-0.23976
63	C(13)	-0.00064	-0.72246	-0.25779	-0.24099
64	C(13)	0.00003	0.03799	0.01356	0.01267
65	C(13)	0.00146	1.64517	0.58704	0.54877
66	C(13)	0.00001	0.01401	0.00500	0.00467
67	C(13)	0.00146	1.63587	0.58372	0.54567
68	C(13)	0.00003	0.03644	0.01300	0.01216
69	H(1)	-0.00001	-0.04364	-0.01557	-0.01456
70	H(1)	-0.00001	-0.02458	-0.00877	-0.00820
71	H(1)	0.00012	0.55587	0.19835	0.18542
72	H(1)	-0.00001	-0.04041	-0.01442	-0.01348
73	H(1)	-0.00001	-0.04272	-0.01524	-0.01425
74	H(1)	0.00000	0.00879	0.00314	0.00293
75	H(1)	-0.00029	-1.29652	-0.46263	-0.43247
76	H(1)	0.00032	1.43664	0.51263	0.47921
77	H(1)	-0.00001	-0.02541	-0.00907	-0.00848
78	H(1)	0.00012	0.55666	0.19863	0.18568
79	H(1)	-0.00001	-0.04349	-0.01552	-0.01451
80	H(1)	-0.00005	-0.24372	-0.08697	-0.08130
81	H(1)	-0.00003	-0.12074	-0.04308	-0.04028
82	H(1)	-0.00001	-0.03154	-0.01125	-0.01052
83	H(1)	-0.00029	-1.30095	-0.46421	-0.43395
84	H(1)	0.00032	1.44342	0.51505	0.48147
85	C(13)	0.00001	0.01444	0.00515	0.00482
86	H(1)	0.00000	0.01445	0.00516	0.00482
87	H(1)	-0.00001	-0.03967	-0.01416	-0.01323
88	H(1)	-0.00001	-0.04190	-0.01495	-0.01398
89	H(1)	-0.00003	-0.12292	-0.04386	-0.04100

90	H(1)	-0.00001	-0.03266	-0.01165	-0.01089
91	H(1)	-0.00006	-0.25105	-0.08958	-0.08374

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