Chelatoaromaticity – Existing: Yes or No? An Answer Given by Spatial Magnetic Properties (Through Space NMR Shieldings – TSNMRS) †

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Supporting Information

Coordinates and absolute energies (a.u.) at the B3LYP/6-311G** level of theory of all studied compounds **4–14**, and visualization of the TSNMRSs of the acetyl acetonato complexes **5b,c** and **6**.

2

Total energies in a.u. and Cartesian coordinates in Å

4

E = -694.9848763 a.u.

1	6	0.234249	0.001237	-0.022790
2	6	0.946236	1.216997	0.026500
3	6	2.342635	1.195309	0.021297
4	6	3.061497	0.001100	-0.030477
5	6	2.342287	-1.192612	-0.088280
6	6	0.945773	-1.214241	-0.084761
7	6	-1.264179	0.000434	0.002838
8	6	0.224575	2.544637	0.066183
9	1	2.882193	2.137434	0.056881
10	6	4.570957	-0.000332	0.000942
11	1	2.881512	-2.134114	-0.139034
12	6	0.223351	-2.539980	-0.165500
13	6	-2.007845	0.053241	-1.159020
14	8	-3.331778	0.053475	-1.155395
15	6	-1.976718	-0.058205	1.272430
16	8	-3.221869	-0.061103	1.330676
17	6	-1.195015	-0.117646	2.566231
18	6	-1.431777	0.115893	-2.539079
19	1	-3.603151	0.010231	-0.185237
20	1	-0.352687	2.715848	-0.847486
21	1	0.933174	3.367990	0.172784
22	1	-0.484620	2.600667	0.896891
23	1	4.941596	-0.040281	1.031129
24	1	4.981101	0.902458	-0.457878
25	1	4.980699	-0.864832	-0.526674
26	1	0.932432	-3.369458	-0.142442
27	1	-0.360756	-2.624305	-1.086830
28	1	-0.479959	-2.675221	0.661108
29	1	-0.545785	0.755570	2.672165
30	1	-0.542316	-0.994552	2.588453
31	1	-1.896789	-0.158781	3.397836
32	1	-1.796278	-0.735772	-3.120902
33	1	-0.344182	0.113990	-2.532740
34	1	-1.793164	1.019148	-3.039362

5a

E = -701.9953259 a.u.

1	6	0.276401	-0.010217	-0.000711
2	6	0.990742	-0.004044	1.214621
3	6	2.387738	0.003582	1.195569
4	6	3.108428	0.001192	0.001804
5	6	2.389858	-0.008438	-1.193769
6	6	0.993370	-0.016337	-1.215165
7	6	-1.228105	0.001439	-0.002269
8	6	0.268429	-0.019571	2.542568
9	1	2.926353	0.012085	2.139092
10	6	4.618550	-0.021402	0.002445
11	1	2.930225	-0.009624	-2.136379
12	6	0.272486	-0.041834	-2.543604
13	6	-1.888952	1.266293	-0.008363
14	8	-3.146154	1.436580	-0.005522
15	6	-1.943911	-1.227136	0.004607
16	8	-3.211022	-1.335967	0.006596
17	6	-1.200735	-2.551010	0.010033
18	6	-1.053216	2.536288	-0.013199
19	3	-4.260606	0.071219	0.003234
20	1	-0.431439	0.815459	2.636941
21	1	0.977474	0.037621	3.371024
22	1	-0.320506	-0.933410	2.666768
23	1	4.997585	-1.048985	-0.031397
24	1	5.024075	0.446196	0.902795
25	1	5.025903	0.504023	-0.864857
26	1	0.983028	-0.004920	-3.371932
27	1	-0.416455	0.801006	-2.650211
28	1	-0.328306	-0.949403	-2.655588
29	1	-1.509747	-3.117278	0.893541
30	1	-0.117309	-2.455791	0.002765
31	1	-1.521256	-3.130611	-0.860526
32	1	-1.723052	3.392263	-0.085578
33	1	-0.343977	2.550870	-0.843973
34	1	-0.459876	2.619097	0.901837

5b

E = -856.7426342 a.u.

1	6	0.560413	-0.000603	0.002106
2	6	1.276559	0.000342	-1.212813
3	6	2.673720	-0.004955	-1.195734
4	6	3.395924	-0.009018	-0.003018
5	6	2.678137	-0.013173	1.192854
6	6	1.281436	-0.008008	1.214829
7	6	-0.945083	0.001333	0.004630
8	6	0.554839	0.003349	-2.541458
9	1	3.211541	-0.007880	-2.139986
10	6	4.906129	0.019152	-0.005345
11	1	3.219428	-0.022584	2.135103
12	6	0.563130	-0.014276	2.545052
13	6	-1.618497	-1.257116	-0.001525
14	8	-2.869052	-1.436354	-0.009099
15	6	-1.614755	1.261759	0.007208
16	8	-2.864758	1.444865	0.001252
17	6	-0.766284	2.531712	0.012074
18	6	-0.773944	-2.529680	-0.005253
19	11	-4.417723	0.006571	-0.012658
20	1	-0.093691	-0.870541	-2.652316
21	1	1.266648	0.002739	-3.369889
22	1	-0.089202	0.880870	-2.649979
23	1	5.282245	1.048238	0.017829
24	1	5.312660	-0.455914	-0.901549
25	1	5.316367	-0.496535	0.866529
26	1	1.276715	-0.019530	3.371937
27	1	-0.084546	-0.889526	2.651145
28	1	-0.081871	0.861814	2.660073
29	1	-0.179734	2.619055	-0.907220
30	1	-0.051336	2.543854	0.838174
31	1	-1.434071	3.389051	0.092114
32	1	-1.444348	-3.385420	0.069815
33	1	-0.058377	-2.549386	0.820140
34	1	-0.188360	-2.613108	-0.925519

5c

E = -1294.3821331 a.u.

1	6	-0.880996	-0.000906	0.001233
2	6	-1.602663	-0.022213	1.213577
3	6	-2.999556	-0.026897	1.192556
4	6	-3.718174	-0.009011	-0.002502
5	6	-2.996470	0.008591	-1.195487
6	6	-1.599358	0.014086	-1.212852
7	6	0.623576	0.000534	0.003124
8	6	-0.884192	-0.041567	2.543603
9	1	-3.540370	-0.047188	2.135017
10	6	-5.228489	0.019523	-0.004008
11	1	-3.534778	0.016592	-2.139568
12	6	-0.878113	0.030455	-2.541543
13	6	1.303588	-1.254572	-0.015702
14	8	2.552143	-1.421750	-0.016904
15	6	1.301400	1.256757	0.020903
16	8	2.549692	1.425991	0.017760
17	6	0.457144	2.532065	0.038963
18	6	0.461020	-2.531060	-0.034830
19	19	4.506154	0.004004	-0.001876
20	1	-0.229841	-0.913060	2.637320
21	1	-1.597689	-0.062772	3.370525
22	1	-0.245471	0.837638	2.669549
23	1	-5.604895	1.048688	0.013618
24	1	-5.638255	-0.491529	0.870843
25	1	-5.635814	-0.460424	-0.897396
26	1	-1.590099	0.041652	-3.369964
27	1	-0.232120	-0.844157	-2.661586
28	1	-0.230824	0.906797	-2.639011
29	1	1.129219	3.385435	0.128487
30	1	-0.258227	2.540005	0.865046
31	1	-0.128612	2.633096	-0.879654
32	1	1.136806	-3.385895	-0.056570
33	1	-0.199152	-2.567758	-0.905652
34	1	-0.183786	-2.601839	0.845575

6

E = -919.1692956 a.u.

1	6	0.985800	-0.030944	-0.001472
2	6	1.621956	1.225983	-0.012817
3	6	3.017481	1.281908	-0.017497
4	6	3.802548	0.129144	-0.009602
5	6	3.153587	-1.106281	-0.002079
6	6	1.761296	-1.208130	0.003334
7	6	-0.510885	-0.105356	0.000732
8	6	0.823563	2.509669	-0.023020
9	1	3.502543	2.253286	-0.029615
10	6	5.309456	0.214285	0.017779
11	1	3.745884	-2.016428	-0.002056
12	6	1.113844	-2.573918	0.011030
13	6	-1.245936	-0.187950	-1.194389
14	8	-2.534510	-0.212527	-1.216279
15	6	-1.242711	-0.169249	1.198965
16	8	-2.531192	-0.192992	1.224756
17	6	-0.604973	-0.237790	2.552010
18	6	-0.611958	-0.277075	-2.548009
19	5	-3.374030	0.108775	0.002856
20	9	-4.469137	-0.698580	0.010953
21	9	-3.642285	1.455612	-0.007631
22	1	0.167509	2.575244	-0.895663
23	1	1.486054	3.376572	-0.036833
24	1	0.178695	2.595160	0.856334
25	1	5.682980	0.200526	1.047519
26	1	5.665232	1.136580	-0.446604
27	1	5.766575	-0.628552	-0.505771
28	1	1.869933	-3.360665	0.011713
29	1	0.473856	-2.727066	-0.862999
30	1	0.480553	-2.719443	0.891270
31	1	0.467644	-0.407999	2.503149
32	1	-1.092420	-1.023030	3.133938
33	1	-0.792881	0.706247	3.073842
34	1	-0.805718	0.656988	-3.085345
35	1	-1.097803	-1.074272	-3.114890
36	1	0.461521	-0.441949	-2.499779

7a

E = -5028.745193 a.u.

1	77	0.092901	0.104353	-0.083713
2	6	1.841021	-0.942692	-0.107367
3	6	3.172232	-0.514668	-0.182612
4	6	3.531498	0.882425	-0.323497
5	6	2.609342	1.939064	-0.412306
6	6	1.174534	1.731644	-0.342431
7	15	-0.398198	-0.846107	2.085877
8	6	4.337213	-1.526542	-0.137125
9	1	4.600428	1.124226	-0.380239
10	6	3.135755	3.376737	-0.602509
11	1	0.661654	2.713409	-0.431093
12	15	-0.823753	-1.684675	-1.492818
13	15	-1.859417	1.630404	-0.197795
14	1	1.756192	-2.044637	-0.014030
15	6	0.448999	0.211709	3.429163
16	6	0.287749	-2.567839	2.559766
17	6	-2.155989	-0.993847	2.840472
18	1	5.001172	-1.343441	0.730310
19	1	4.969184	-1.462085	-1.044024
20	1	3.963437	-2.562762	-0.061034
21	1	4.238658	3.401724	-0.650172
22	1	2.820309	4.037720	0.228114
23	1	2.749485	3.826563	-1.537556
24	6	-2.637397	-1.715970	-2.103235
25	6	-0.632881	-3.538391	-1.037765
26	6	0.084114	-1.666477	-3.170540
27	6	-1.822487	3.045359	1.085533
28	6	-3.685702	1.091890	-0.009210
29	6	-1.991557	2.634665	-1.816148
30	1	0.313593	-0.224057	4.434856
31	1	0.029665	1.228649	3.399677
32	1	1.517757	0.272652	3.179014
33	1	0.119538	-2.761659	3.633127
34	1	1.365394	-2.587785	2.343272
35	1	-0.211165	-3.347371	1.964692
36	1	-2.106319	-1.424984	3.855354
37	1	-2.778170	-1.638324	2.199522
38	1	-2.617253	0.004557	2.898518
39	1	-2.874525	-0.753806	-2.583093
40	1	-3.316466	-1.868867	-1.249796
41	1	-2.783999	-2.528409	-2.835288
42	1	0.401371	-3.728552	-0.714885
43	1	-0.867033	-4.178476	-1.905634
44	1	-1.318920	-3.782429	-0.210818
45	1	-0.070458	-0.682508	-3.637891
46	1	1.159302	-1.782642	-2.971801
47	1	-0.275375	-2.468201	-3.840000
48	1	-2.603545	3.795740	0.875123
49	1	-0.831245	3.520435	1.061176
50	1	-1.982230	2.622417	2.090312
51	1	-4.340384	1.978118	0.041319
52	1	-3.805645	0.498891	0.909082
53	1	-3.984050	0.474391	-0.868533
54	1	-2.805433	3.378505	-1.766728
55	1	-2.174425	1.939504	-2.650645
56	1	-1.032017	3.141549	-1.994401

8

E = -1891.9951756 a.u.

1	44	-1.220936	-0.000065	0.000035
2	7	0.382506	1.349202	-0.040434
3	6	1.660673	0.727166	-0.059182
4	6	2.911295	1.414814	-0.143690
5	6	1.660687	-0.727162	0.059377
6	7	0.382536	-1.349193	0.040828
7	7	-0.917144	0.266179	2.162471
8	6	4.150304	0.707350	-0.078368
9	7	-0.916832	-0.266049	-2.162321
10	6	4.150317	-0.707346	0.078167
11	7	-2.726449	1.701659	-0.131236
12	7	-2.726597	-1.701539	0.130770
13	6	2.911324	-1.414814	0.143685
14	1	0.406932	2.331514	-0.348751
15	1	2.909729	2.507480	-0.240264
16	1	0.407005	-2.331571	0.348928
17	1	-1.650741	0.529132	2.830042
18	1	-0.236266	1.033661	2.000797
19	1	-0.420731	-0.578043	2.475749
20	1	5.094096	1.258445	-0.140104
21	1	-1.650358	-0.529161	-2.829932
22	1	-0.420631	0.578296	-2.475616
23	1	-0.235748	-1.033390	-2.000871
24	1	5.094122	-1.258438	0.139742
25	1	-3.195627	1.737963	-1.041484
26	1	-2.127533	2.527113	-0.016980
27	1	-3.426224	1.675891	0.618021
28	1	-3.198143	-1.736760	1.039844
29	1	-3.424444	-1.676292	-0.620299
30	1	-2.127756	-2.527377	0.018900
31	1	2.909775	-2.507480	0.240258

9

E = -2659.1807544 a.u.

1	44	-0.000058	0.006664	-0.005428
2	7	0.023603	2.065476	0.036680
3	6	-0.004576	2.702959	-1.201277
4	6	-0.020143	4.119955	-1.425893
5	6	0.004084	1.796926	-2.349587
6	7	-0.024154	0.444603	-2.017600
7	7	2.071950	-0.162934	-0.062054
8	6	-0.013587	4.638611	-2.748585
9	7	-2.072020	0.021821	0.172994
10	6	0.013238	3.752109	-3.872149
11	7	-0.251780	-0.128041	2.081953
12	7	0.251973	-2.054864	-0.359360
13	6	0.019725	2.345040	-3.675439
14	1	-0.109646	2.665468	0.857479
15	1	-0.034525	4.797902	-0.565753
16	6	-2.580250	0.098451	1.473649
17	6	-3.990841	0.161794	1.705207
18	6	-4.881030	0.179240	0.611847
19	1	-0.027174	5.721054	-2.906107
20	6	-4.346013	0.140588	-0.715682
21	6	-2.947432	0.059304	-0.885482
22	6	-1.564091	0.056928	2.534875
23	1	0.026897	4.157126	-4.888246
24	6	-1.850869	0.149514	3.934205
25	6	-0.810267	0.018949	4.876176
26	6	0.522199	-0.212702	4.404863
27	6	0.748690	-0.270626	3.013067
28	6	1.564334	-2.452218	-0.644584
29	6	1.851321	-3.791764	-1.059521
30	1	0.034100	1.666226	-4.534894
31	6	0.810888	-4.738514	-1.151105
32	6	-0.521616	-4.334109	-0.816227
33	6	-0.748334	-2.993825	-0.436760
34	6	2.580343	-1.410161	-0.438682
35	6	2.947215	0.875438	0.147215
36	6	4.345816	0.729379	0.028592
37	6	4.881007	-0.552777	-0.317366
38	6	3.990955	-1.620436	-0.554233
39	1	0.109325	-0.214039	-2.792092
40	1	-4.375499	0.194473	2.724903
41	1	-5.958993	0.229972	0.777449
42	1	-4.994694	0.188169	-1.590749
43	1	-2.471881	0.046571	-1.865768
44	1	-2.873269	0.325495	4.269540
45	1	-1.019063	0.092163	5.945213
46	1	1.356851	-0.334582	5.095796
47	1	1.748174	-0.423843	2.606700
48	1	2.873757	-4.076904	-1.308596
49	1	1.019854	-5.761314	-1.470496
50	1	-1.356142	-5.034617	-0.857990
51	1	-1.747852	-2.634331	-0.193234
52	1	2.471584	1.825912	0.387317
53	1	4.994360	1.591676	0.185514
54	1	5.958982	-0.701920	-0.405260
55	1	4.375745	-2.604597	-0.822882

11

E = -418.6811208 a.u.

1	6	-0.573338	0.809164	-0.000131
2	6	-0.605778	-0.661749	0.000026
3	6	0.536161	-1.381004	-0.000002
4	8	1.763885	-0.782158	-0.000014
5	6	1.837890	0.557893	-0.000005
6	6	0.758821	1.370826	0.000039
7	8	-1.640051	1.427290	0.000011
8	8	-1.827983	-1.218990	0.000045
9	1	0.603596	-2.458807	-0.000053
10	1	-2.444458	-0.460299	-0.000085
11	1	2.866871	0.892900	0.000072
12	1	0.884647	2.446292	0.000167

12

E = -1496.9830695 a.u.

1	8	2.546167	4.316514	-0.513059
2	6	2.365369	3.107504	-1.121488
3	6	1.512521	2.163793	-0.614762
4	6	0.789618	2.486946	0.612184
5	6	1.014156	3.759029	1.202612
6	6	1.888070	4.613526	0.604430
7	1	2.956337	3.003446	-2.017638
8	8	1.271257	0.989242	-1.112519
9	8	0.009920	1.591799	1.048778
10	13	-0.001353	-0.000482	-0.128519
11	1	0.502045	4.043666	2.111931
12	1	2.133190	5.601989	0.967544
13	8	2.473505	-4.358799	-0.513898
14	6	1.516324	-3.599255	-1.123309
15	6	1.120507	-2.391067	-0.615051
16	6	1.757910	-1.927009	0.614144
17	6	2.748164	-2.755785	1.205459
18	6	3.055916	-3.937935	0.605854
19	1	1.134156	-4.058448	-2.021224
20	8	0.222732	-1.596551	-1.113309
21	8	1.368593	-0.805857	1.051795
22	1	3.247776	-2.454783	2.116456
23	1	3.790418	-4.643151	0.969393
24	8	-5.013606	0.042259	-0.514008
25	6	-3.876526	0.490215	-1.123149
26	6	-2.632558	0.226034	-0.615576
27	6	-2.550496	-0.559215	0.612760
28	6	-3.763910	-1.001200	1.203758
29	6	-4.941176	-0.673997	0.604922
30	1	-4.082343	1.052398	-2.020220
31	8	-1.495076	0.605280	-1.113346
32	8	-1.385245	-0.784725	1.050217
33	1	-3.753797	-1.585371	2.114127
34	1	-5.919505	-0.956283	0.968453

13

E = -1106.1565723 a.u.

1	6	-0.791923	-0.015169	0.000848
2	6	-1.628271	0.955523	0.572631
3	6	-3.005642	0.767527	0.612905
4	6	-3.575290	-0.385576	0.075568
5	6	-2.756174	-1.349400	-0.507526
6	6	-1.377442	-1.164236	-0.550466
7	6	0.683947	0.149923	-0.010788
8	6	1.490742	-0.875485	0.313552
9	16	3.262013	-0.866331	0.173940
10	16	1.244196	1.775362	-0.493918
11	1	-1.191440	1.849691	1.000297
12	1	-3.635718	1.523347	1.068132
13	1	-4.649697	-0.527134	0.103564
14	1	-3.191156	-2.241946	-0.943127
15	1	-0.746695	-1.900590	-1.034232
16	1	1.050095	-1.808896	0.640797
17	1	3.510738	-1.561145	1.303186
18	1	2.514831	1.623542	-0.059318

14a

E = -4459.2915663 a.u.

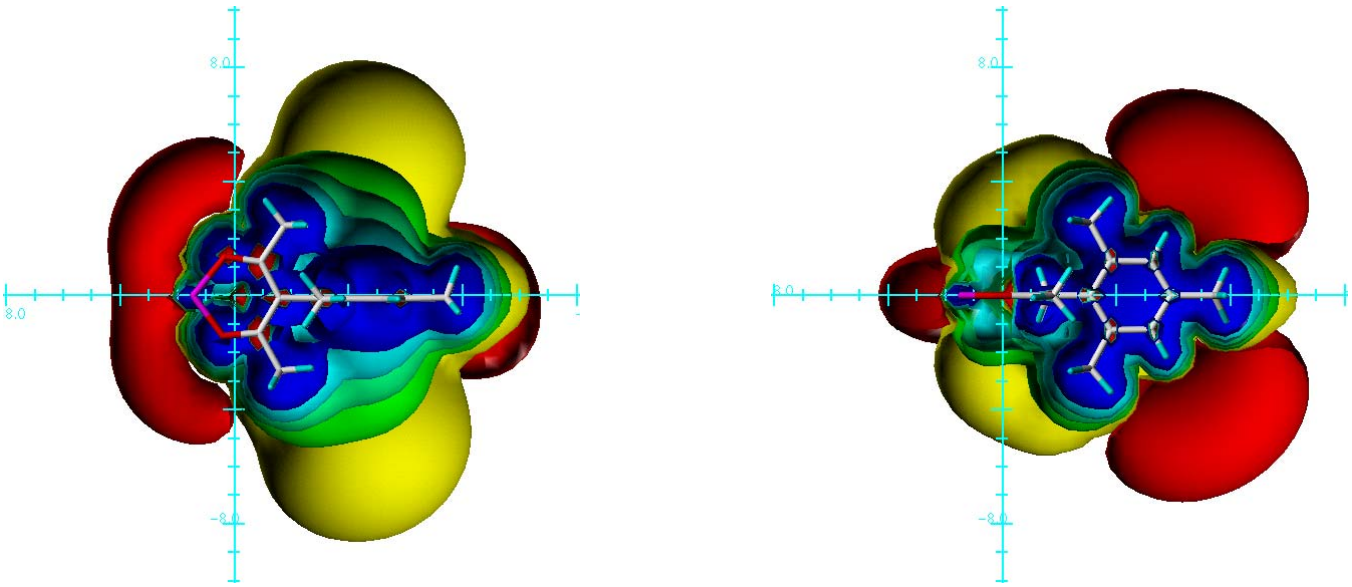
1	6	2.925866	-3.825200	-0.003936
2	6	3.107206	-4.108806	-1.396367
3	6	3.973019	-5.153828	-1.812906
4	6	4.678101	-5.929971	-0.851075
5	6	4.513112	-5.649504	0.535433
6	6	3.648056	-4.607710	0.957859
7	6	2.001425	-2.734388	0.445586
8	6	1.371077	-2.732731	1.692893
9	16	0.338385	-1.393857	2.252058
10	16	1.749098	-1.304593	-0.639337
11	1	2.559305	-3.526825	-2.138548
12	1	4.092054	-5.361385	-2.879048
13	1	5.344570	-6.733696	-1.173576
14	1	5.061248	-6.230843	1.281131
15	1	3.559886	-4.382537	2.022194
16	1	1.499158	-3.548344	2.406901
17	42	-0.133193	-0.016039	0.269757
18	6	-4.957448	-0.369911	-0.465603
19	6	-5.612415	-0.966345	0.660420
20	6	-7.028221	-0.971918	0.750011
21	6	-7.817073	-0.372605	-0.272518
22	6	-7.175681	0.237864	-1.387147
23	6	-5.760044	0.242370	-1.484826
24	6	-3.464045	-0.378265	-0.589311
25	6	-2.809255	-0.366644	-1.824327
26	16	-1.036748	-0.427590	-1.979711
27	16	-2.452854	-0.491768	0.911691
28	1	-5.016504	-1.431678	1.446597
29	1	-7.511234	-1.440044	1.611098
30	1	-8.907359	-0.375258	-0.199144
31	1	-7.771746	0.715098	-2.169053
32	1	-5.280821	0.744396	-2.327243
33	1	-3.357493	-0.410433	-2.767316
34	6	2.282543	4.225767	-0.036516
35	6	3.324088	4.040424	-1.002475
36	6	4.188720	5.112978	-1.344949
37	6	4.027205	6.389336	-0.736988
38	6	2.988065	6.587189	0.216618
39	6	2.122111	5.518824	0.564355
40	6	1.375148	3.095483	0.344040
41	6	0.746730	3.007967	1.589642
42	16	-0.405606	1.715008	2.001186
43	16	1.009474	1.819907	-0.890334
44	1	3.462760	3.060666	-1.461361
45	1	4.983555	4.950923	-2.076985
46	1	4.693650	7.213701	-1.002430
47	1	2.846965	7.567856	0.677941
48	1	1.308342	5.695326	1.270010
49	1	0.910019	3.750750	2.372720

14b

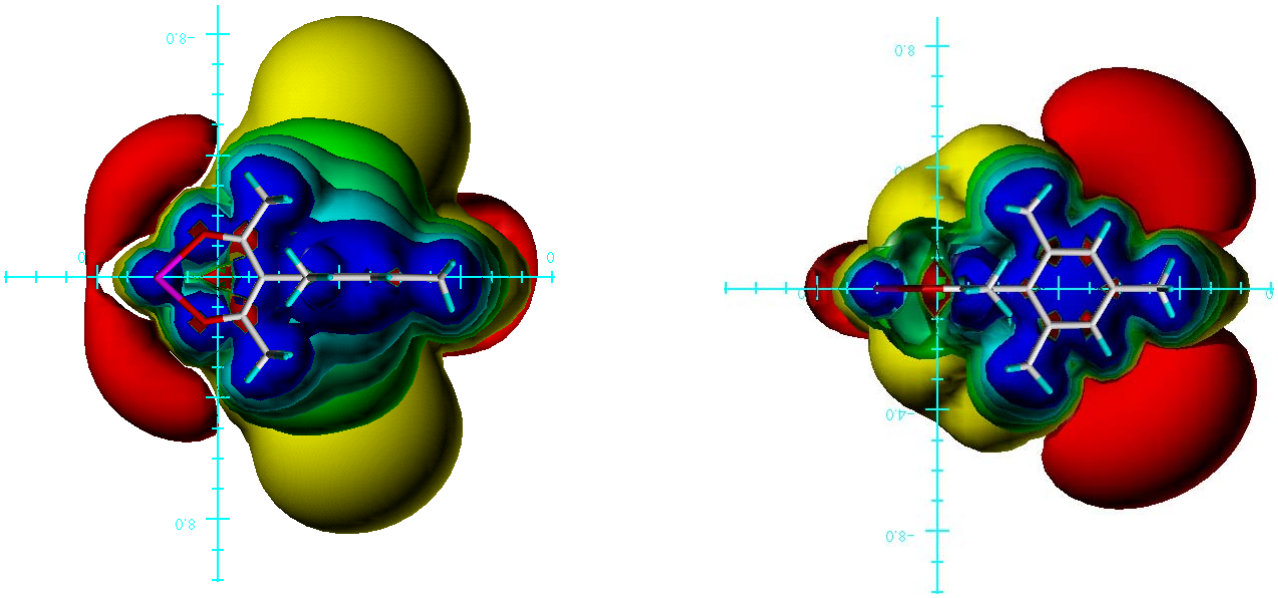
E = -4258.9882967 a.u.

1	6	2.782566	-3.715036	0.015198
2	6	2.919642	-4.024041	-1.348194
3	6	3.745477	-5.061210	-1.770006
4	6	4.459628	-5.818492	-0.843451
5	6	4.342709	-5.518888	0.513284
6	6	3.521328	-4.479363	0.935908
7	6	1.895706	-2.620790	0.466177
8	6	1.256969	-2.636462	1.673077
9	16	0.314168	-1.304727	2.222535
10	16	1.719015	-1.198147	-0.536075
11	1	2.361113	-3.443049	-2.071353
12	1	3.827259	-5.280760	-2.829576
13	1	5.103715	-6.626681	-1.173471
14	1	4.904794	-6.088786	1.246290
15	1	3.467689	-4.236196	1.990629
16	1	1.349519	-3.476659	2.353194
17	23	-0.139347	-0.011891	0.290349
18	6	-4.801648	-0.313834	-0.440932
19	6	-5.473418	-0.988188	0.592589
20	6	-6.861172	-0.974572	0.675348
21	6	-7.620502	-0.281220	-0.266460
22	6	-6.969552	0.405303	-1.289668
23	6	-5.580686	0.393530	-1.372997
24	6	-3.326931	-0.346208	-0.551929
25	6	-2.683896	-0.318416	-1.756735
26	16	-0.972570	-0.457923	-1.878899
27	16	-2.355787	-0.549120	0.888634
28	1	-4.889561	-1.525736	1.329381
29	1	-7.352654	-1.509582	1.481562
30	1	-8.703076	-0.267805	-0.197777
31	1	-7.544328	0.965183	-2.020507
32	1	-5.086956	0.960007	-2.153838
33	1	-3.234715	-0.312834	-2.691550
34	6	2.239924	4.060902	-0.018546
35	6	3.306970	3.844550	-0.905987
36	6	4.183067	4.872804	-1.238800
37	6	4.018200	6.146196	-0.697123
38	6	2.958389	6.380513	0.178082
39	6	2.079253	5.354728	0.508160
40	6	1.314282	2.966679	0.346379
41	6	0.701629	2.891662	1.564641
42	16	-0.454455	1.669782	1.929193
43	16	0.903874	1.762807	-0.853202
44	1	3.443872	2.854731	-1.323116
45	1	5.002331	4.675274	-1.922443
46	1	4.701876	6.947104	-0.958064
47	1	2.806726	7.370790	0.595640
48	1	1.240141	5.559591	1.162774
49	1	0.891710	3.625281	2.341142

Visualization of the spatial magnetic properties (TSNMRS) of **5a** as ICSS of different direction and size (blue represents 5 ppm shielding, cyan 2 ppm shielding, greenblue 1 ppm shielding, green 0.5 ppm shielding, yellow 0.1 ppm shielding and red –0.1 ppm deshielding)



Visualization of the spatial magnetic properties (TSNMRS) of **5b** as ICSS of different direction and size (blue represents 5 ppm shielding, cyan 2 ppm shielding, greenblue 1 ppm shielding, green 0.5 ppm shielding, yellow 0.1 ppm shielding and red –0.1 ppm deshielding)



Visualization of the spatial magnetic properties (TSNMRS) of **6** as ICSS of different direction and size (blue represents 5 ppm shielding, cyan 2 ppm shielding, greenblue 1 ppm shielding, green 0.5 ppm shielding, yellow 0.1 ppm shielding and red –0.1 ppm deshielding)