Supplementary Information

Understanding the *g*-tensors of Perchlorotriphenylmethyl and Finland-type Trityl radicals

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1 – Synthesis

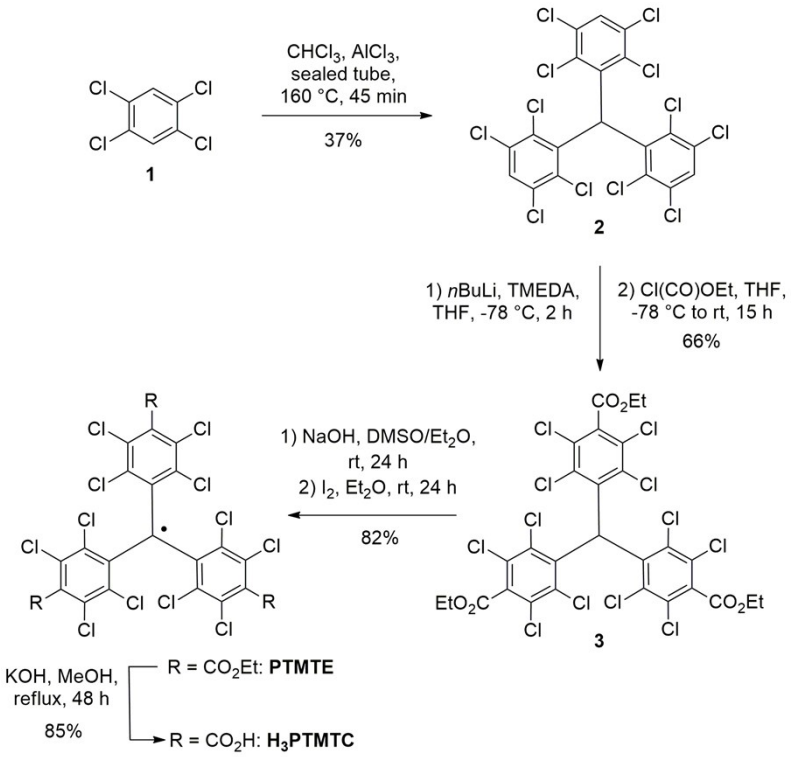
2 – Comparison between X-ray crystallography and DFT calculations

3 – Final optimized DFT structures and calculated g-tensors

4 – Full size reproduction of Figure 4

1 – Synthesis

The tripotassium salt of Finland trityl (FT) was synthesized according to a literature procedure (*J. Org. Chem.* **2002**, *67*, 4635–4639). H_3PTMTC and PTMTE were synthesized according to Scheme S1. We were unable to obtain triarylmethane **2** in a pure form following the described conditions (*Synthesis* **1986**, 64–66) as the retention times of compounds **1** and **2** were very similar. Careful purification by column chromatography using a large amount of silica gel followed by pentane washings allowed the isolation of pure compound **2** in 37% yield. Compound **2** was then converted to PTMTE in two steps (*Bioorg. Med. Chem. Lett.* **2007**, *17*, 4062–4065). The hydrolysis of PTMTE proved more difficult than expected, affording H_3PTMTC at a very slow rate (two weeks) in standard (KOH, H_2O/THF) conditions. The use of other bases (NaOH, LiOH) did not improve the saponification rate. This problem was solved using refluxing methanolic KOH, giving H_3PTMTC in 85% yield in 48 h.



Scheme S1. Synthesis of PTMTE and H_3PTMTC.

2 – Comparison between X-ray crystallography and DFT calculations

A comparison of selected bond lengths and blade angles from DFT calculations and X-ray structures (when available) of PTM and TAM radicals is provided in Table S2. The molecular structures of the PTM radicals as optimized by DFT calculations were in excellent agreement with the X-ray crystallographic structural determinations that have been reported in the literature. As the crystal structures of FT and H_3FT have not been reported, we have included instead the values for Me_3FT in Table S2 for comparison. The molecular structure of H_3FT from the calculations was also an excellent match for the core of the crystal structure of Me_3FT. Interestingly, the blade angles of the aromatic rings were able to be reproduced, with those of the PTM radicals being consistently more twisted from the central plane than the TAM radicals.

Table S2. Comparison of selected bond lengths and blade angles from DFT calculations and X-ray structures (when available) of PTM and TAM radicals discussed in this work.

	PTMTC		H_3PTMTC		FT	H_3FT	Me_3FT
Mean bond length (Å)	DFT	X-ray[a]	DFT	X-ray[b]	DFT	DFT	X-ray[d]
$C_{central}$-C_1	1.479	1.473	1.481	1.473	1.474	1.473	1.449
C_1-$C_{2,6}$	1.419	1.405	1.419	1.407	1.4223	1.422	1.417
$C_{2,6}$-$C_{3.5}$	1.399	1.380	1.401	1.395	1.405	1.406	1.395
$C_{3,5}$-C_4	1.398	1.379	1.397	1.396	1.406	1.414	1.407
$C_{2,6}$-Cl/S	1.749	1.728	1.741	1.724	1.780	1.776	1.758
$C_{3,5}$-Cl/S	1.755	1.728	1.742	1.718	1.784	1.777	1.767
C_4-C_{COOR}	1.542	1.520	1.510	1.502	1.524	1.480	1.480
C=O	1.255	1.223	1.208	1.237	1.263	1.219	1.207
C–O			1.346	1.288		1.355	1.335
Mean blade angle (°)	49.28	48.3	49.48	49.37	46.0	45.6	44.16
Mean C_4-C_{COOR} dihedral angle (°)	89.35	84.0	89.14	86.91	30.4	22.9	17.77

[a]from *CrystEngComm* **2004**, *6*, 573–578, [b]from *Chem. Eur. J.* **2007**, *13*, 8153–8163, [c]calculation performed on the methyl ester derivative, and [d]from *J. Org. Chem.* **2008**, *73*, 1490–1497.

3 – Final optimized DFT structures and calculated g-tensors

A - FT

1	6	3.630527	0.429146	3.096547
2	16	4.810059	-0.504689	2.003207
3	6	3.551903	-1.084437	0.879178
4	6	2.350039	-0.356075	0.859886
5	16	2.277538	1.028436	1.977427
6	6	1.271869	-0.727504	0.009718
7	6	1.482708	-1.854854	-0.832998
8	6	2.689009	-2.575101	-0.805767
9	6	3.739553	-2.205928	0.052226
10	16	2.801982	-3.969555	-1.913619
11	6	1.48035	-3.359638	-3.070007
12	16	0.273076	-2.432718	-2.007645
13	6	0.000016	0.013317	-0.000051
14	6	-1.272945	-0.725581	-0.009774
15	6	-1.485556	-1.852459	0.833146
16	6	-2.69295	-2.57087	0.80601
17	6	-3.742891	-2.200255	-0.052116
18	6	-3.553505	-1.079183	-0.879215
19	6	-2.350537	-0.352642	-0.860018
20	16	-2.80813	-3.964887	1.914185
21	6	-1.485571	-3.356756	3.07047
22	16	-0.276856	-2.431931	2.007964
23	16	-2.27596	1.031575	-1.977803
24	6	-3.629804	0.434111	-3.096818
25	16	-4.810792	-0.497662	-2.003283
26	6	5.041089	-2.997115	0.086095
27	8	6.089057	-2.347644	0.361166
28	6	-5.045664	-2.98938	-0.085925
29	8	-4.962706	-4.224969	0.16233
30	6	-0.778543	-4.557164	3.708609
31	6	-2.082731	-2.432785	4.139495
32	6	-4.34719	1.642175	-3.708234
33	6	-3.064009	-0.484204	-4.187518
34	6	0.77147	-4.559091	-3.707877
35	6	2.078874	-2.4368	-4.139236
36	6	3.063347	-0.488035	4.187465
37	6	4.349755	1.636264	3.707657
38	6	0.001146	1.490226	-0.000087
39	6	0.786914	2.235527	-0.920911
40	6	0.771181	3.64114	-0.929482
41	6	0.003333	4.366086	-0.000124
42	6	-0.765583	3.642339	0.929283
43	6	-0.783463	2.236756	0.920741

44	16	1.710369	4.434742	-2.219997
45	6	2.751512	2.944705	-2.620186
46	16	1.693916	1.469402	-2.243519
47	16	-1.703549	4.437409	2.219787
48	6	-2.746943	2.948972	2.620035
49	16	-1.691616	1.472037	2.243363
50	6	0.004457	5.889476	-0.000175
51	8	0.208465	6.453488	-1.111642
52	6	4.023397	2.925347	-1.762038
53	6	3.093661	2.954582	-4.11426
54	6	-4.018876	2.931526	1.761917
55	6	-3.089033	2.959389	4.114119
56	8	4.956146	-4.232596	-0.161991
57	8	-0.198723	6.453861	1.111257
58	8	-6.092595	-2.338279	-0.361125
59	1	2.355419	0.065098	4.814579
60	1	2.54407	-1.34749	3.755531
61	1	3.876508	-0.856774	4.822612
62	1	3.659525	2.207778	4.337187
63	1	5.172408	1.295524	4.345393
64	1	4.753722	2.298583	2.938461
65	1	1.482449	-5.134305	-4.310503
66	1	0.33704	-5.219142	-2.953481
67	1	-0.02509	-4.215817	-4.376515
68	1	2.804278	-2.990918	-4.745357
69	1	1.288281	-2.061859	-4.798649
70	1	2.587428	-1.580768	-3.688199
71	1	-2.809011	-2.98568	4.745683
72	1	-1.291606	-2.058917	4.798882
73	1	-2.589965	-1.57607	3.688267
74	1	-1.490401	-5.131156	4.311362
75	1	-0.345123	-5.218045	2.954358
76	1	0.01855	-4.214969	4.377167
77	1	-3.877732	-0.851908	-4.822545
78	1	-2.355295	0.06773	-4.8148
79	1	-2.545971	-1.344306	-3.755381
80	1	-5.170393	1.302535	-4.345843
81	1	-4.750102	2.305331	-2.939204
82	1	-3.656098	2.212446	-4.337946
83	1	-4.619585	3.823703	1.971195
84	1	-3.780977	2.915775	0.695089
85	1	-4.618736	2.04484	1.995383
86	1	-3.68772	3.845065	4.351973
87	1	-3.687136	2.078735	4.370868
88	1	-2.190049	2.967478	4.734611
89	1	3.693747	3.839317	-4.352092
90	1	3.690391	2.072992	-4.370993
91	1	2.194715	2.964081	-4.734788

92	1	4.625413	3.816651	-1.971271
93	1	3.785458	2.909884	-0.695214
94	1	4.621956	2.03779	-1.995535

g value of the free electron [g_e]: 0.20023193D+01

relativistic mass correction [g_RMC]: -0.16308623D-03

diamagnetic correction to g tensor [g_DC]:

XX= 0.54730466D-04 YX=-0.54975364D-07 ZX=-0.87553638D-04

XY=-0.49583337D-07 YY=-0.14902175D-04 ZY= 0.88925985D-07

XZ= 0.79756642D-04 YZ=-0.59037939D-07 ZZ= 0.12455007D-05

orbital Zeeman and spin-orbit coupling contribution to g tensor [g_OZ/SOC]:

XX= 0.57117772D-03 YX= 0.42787727D-06 ZX=-0.30424271D-03

XY= 0.68968763D-06 YY= 0.10545503D-02 ZY= 0.43861297D-06

XZ=-0.47395591D-03 YZ= 0.32825424D-06 ZZ= 0.43424304D-03

g tensor [g = g_e + g_RMC + g_DC + g_OZ/SOC]:

XX= 0.20027821D+01 YX= 0.37290191D-06 ZX=-0.39179635D-03

XY= 0.64010429D-06 YY= 0.20031959D+01 ZY= 0.52753895D-06

XZ=-0.39419927D-03 YZ= 0.26921630D-06 ZZ= 0.20025917D+01

g shifts relative to the free electron (ppm):

xx= -36.8 yy= 772.0 zz= 876.6

B – H_3FT

1	16	1.595148	1.56571	-2.23117
2	6	0.641524	2.277956	-0.91511
3	6	0.54275	3.68139	-0.92293
4	16	1.47989	4.510517	-2.18722
5	6	2.606745	3.082216	-2.55617
6	6	-0.09623	1.484021	0.004147
7	6	-0.92864	2.162994	0.932728
8	6	-1.01369	3.566626	0.949493
9	6	-0.28961	4.340372	0.01326
10	16	-2.01433	4.273664	2.233761
11	6	-2.94335	2.710675	2.62145
12	16	-1.76898	1.326608	2.251053
13	6	0.000329	0.010154	-0.00273
14	6	1.317995	-0.64515	0.005984
15	6	1.591714	-1.76095	-0.83459
16	6	2.837652	-2.41142	-0.81129
17	6	3.858761	-1.96321	0.058512
18	6	3.613692	-0.84061	0.880462
19	6	2.366996	-0.19162	0.851679
20	16	3.020893	-3.77284	-1.94388
21	6	1.661403	-3.23818	-3.08631
22	16	0.411749	-2.40337	-2.00077
23	16	2.20428	1.19817	1.945337
24	6	3.586822	0.703649	3.077132
25	16	4.821346	-0.16918	1.99805
26	6	5.19169	-2.60572	0.12924
27	8	6.21168	-2.03337	0.482518
28	6	1.025347	-4.47827	-3.72362
29	6	2.195206	-2.27175	-4.15008
30	6	4.232814	1.963773	3.662447
31	6	3.078071	-0.23028	4.181589
32	6	-0.42232	5.814571	0.077017
33	8	-0.14082	6.440893	-1.083
34	6	-4.20195	2.602415	1.752075
35	6	-3.29051	2.694591	4.114145
36	6	3.842189	3.119823	-1.64897
37	6	2.996715	3.123262	-4.03772
38	6	-1.22471	-0.80618	-0.01259
39	6	-2.32293	-0.484	-0.85825
40	6	-3.48747	-1.27098	-0.88404
41	6	-3.59919	-2.40564	-0.04671
42	6	-2.52074	-2.73735	0.803424
43	6	-1.35652	-1.9495	0.822706
44	16	-2.31327	0.908003	-1.96361
45	6	-3.60483	0.237905	-3.11078
46	16	-4.74504	-0.75269	-2.03366

47	16	-2.53867	-4.13636	1.898366
48	6	-1.23376	-3.47401	3.040968
49	16	-0.10247	-2.46548	1.972097
50	6	-2.97112	-0.64755	-4.18994
51	6	-4.38345	1.404182	-3.72857
52	6	-4.79513	-3.27965	-0.0335
53	8	-4.78268	-4.45508	0.299298
54	6	-0.44843	-4.6465	3.638303
55	6	-1.86514	-2.60618	4.136226
56	8	-5.93177	-2.65387	-0.40176
57	8	5.185373	-3.91044	-0.211
58	8	-0.77419	6.428641	1.073234
59	1	-2.28467	-0.05353	-4.80277
60	1	-2.41106	-1.47579	-3.74914
61	1	-3.75185	-1.05997	-4.8383
62	1	-3.71382	2.016553	-4.34116
63	1	-5.1724	1.020728	-4.38393
64	1	-4.83791	2.037084	-2.96322
65	1	-1.11408	-5.26969	4.244624
66	1	0.003656	-5.26663	2.861219
67	1	0.342741	-4.27199	4.296117
68	1	-2.55106	-3.21052	4.739909
69	1	-1.08494	-2.20391	4.791332
70	1	-2.42345	-1.76896	3.709976
71	1	2.951576	-2.77403	-4.76298
72	1	1.377575	-1.94548	-4.80181
73	1	2.647935	-1.38739	-3.69515
74	1	1.763541	-5.00082	-4.34094
75	1	0.644202	-5.16919	-2.9686
76	1	0.19991	-4.18006	-4.37823
77	1	3.912291	-0.53733	4.821838
78	1	2.336656	0.289324	4.798024
79	1	2.612378	-1.12621	3.76366
80	1	5.073258	1.68599	4.307053
81	1	4.5965	2.632225	2.878961
82	1	3.507786	2.504539	4.279515
83	1	4.405099	4.042493	-1.82745
84	1	3.565023	3.078819	-0.5928
85	1	4.492106	2.26608	-1.86849
86	1	3.565136	4.035064	-4.24801
87	1	3.640651	2.270831	-4.27719
88	1	2.119539	3.097228	-4.68787
89	1	-3.9567	3.531056	4.349659
90	1	-3.8205	1.770157	4.365741
91	1	-2.39704	2.770485	4.737668
92	1	-4.86822	3.447233	1.95811
93	1	-3.95478	2.605877	0.687588
94	1	-4.73532	1.673332	1.980151

95	1	6.101766	-4.23727	-0.18077
96	1	-6.6505	-3.31025	-0.40938
97	1	-0.21298	7.400379	-0.93571

g value of the free electron [g_e]: 0.20023193D+01

relativistic mass correction [g_RMC]:-0.16347915D-03

diamagnetic correction to g tensor [g_DC]:

XX= 0.41082783D-04 YX= 0.14546571D-04 ZX=-0.11924377D-03

XY= 0.16745123D-04 YY=-0.47093066D-04 ZY=-0.82578940D-05

XZ= 0.10930791D-03 YZ= 0.10827694D-04 ZZ= 0.23392070D-04

orbital Zeeman and spin-orbit coupling contribution to g tensor [g_OZ/SOC]:

XX= 0.61974153D-03 YX=-0.58570480D-04 ZX=-0.11833771D-03

XY=-0.13796902D-04 YY= 0.13138458D-02 ZY= 0.40259604D-04

XZ=-0.64979994D-03 YZ=-0.10621632D-03 ZZ= 0.12418271D-02

g tensor [g = g_e + g_RMC + g_DC + g_OZ/SOC]:

XX= 0.20028166D+01 YX=-0.44023909D-04 ZX=-0.23758147D-03

XY= 0.29482207D-05 YY= 0.20034226D+01 ZY= 0.32001710D-04

XZ=-0.54049203D-03 YZ=-0.95388628D-04 ZZ= 0.20034210D+01

g shifts relative to the free electron (ppm):

xx= 305.6 yy= 1102.6 zz= 1294.2

C – PTMTC

1	6	0.536171	2.302923	0.910245
2	6	0.794367	1.246874	-0.00208
3	6	1.861817	1.454149	-0.9142
4	6	2.618366	2.631043	-0.89964
5	6	2.344058	3.667315	-0.00212
6	6	1.288482	3.48245	0.895794
7	6	-0.00198	0.000269	-0.00093
8	6	-1.47985	0.066097	-0.00053
9	6	-2.26386	-0.68418	0.914098
10	6	-3.66157	-0.62449	0.899787
11	6	-4.35067	0.193363	-0.00065
12	6	-3.59179	0.947539	-0.90065
13	6	-2.19428	0.883029	-0.91503
14	17	-1.48633	-1.63215	2.161087
15	17	-4.59949	-1.56546	2.04655
16	6	-5.89125	0.261574	-0.00053
17	8	-6.46645	-0.57528	-0.73804
18	17	-4.44248	1.969872	-2.04581
19	17	-1.3356	1.759423	-2.16112
20	17	2.192937	0.269861	-2.15762
21	17	3.933113	2.852163	-2.04095
22	6	3.176117	4.965925	-0.00168
23	8	4.189932	4.954559	0.737974
24	17	0.941372	4.767484	2.039605
25	17	-0.67621	2.107782	2.155401
26	6	0.679853	-1.31253	0.000842
27	6	0.328692	-2.3414	-0.91128
28	6	0.973312	-3.58314	-0.89681
29	6	2.008295	-3.86098	0.001214
30	6	2.372398	-2.85371	0.899773
31	6	1.723568	-1.61427	0.913949
32	17	-0.86251	-2.039	-2.15533
33	17	2.157177	-0.46467	2.158451
34	17	3.660067	-3.1913	2.043441
35	6	2.721917	-5.22814	0.000805
36	8	3.734218	-5.30607	-0.73696
37	17	0.51298	-4.83292	-2.03975
38	8	2.741884	5.88325	-0.73992
39	8	-6.39017	1.145105	0.737956
40	8	2.207028	-6.10367	0.737819

g value of the free electron [g_e]: 0.20023193D+01
relativistic mass correction [g_RMC]: -0.17116759D-03
diamagnetic correction to g tensor [g_DC]:
XX= 0.49422686D-04 YX=-0.28164798D-07 ZX=-0.95618067D-08
XY=-0.58524774D-07 YY= 0.49034845D-04 ZY= 0.29245435D-06

XZ=-0.69329489D-06 YZ=-0.83187127D-06 ZZ= 0.14325631D-04
orbital Zeeman and spin-orbit coupling contribution to g tensor [g_OZ/SOC]:
XX=-0.70739929D-03 YX= 0.57219596D-05 ZX=-0.57616206D-05
XY=-0.36615073D-05 YY=-0.71620186D-03 ZY= 0.20925243D-04
XZ=-0.13337173D-05 YZ=-0.18809685D-06 ZZ= 0.22633103D-02
g tensor [g = g_e + g_RMC + g_DC + g_OZ/SOC]:
XX= 0.20014902D+01 YX= 0.56937948D-05 ZX=-0.57711824D-05
XY=-0.37200321D-05 YY= 0.20014810D+01 ZY= 0.21217697D-04
XZ=-0.20270122D-05 YZ=-0.10199681D-05 ZZ= 0.20044258D+01
g shifts relative to the free electron (ppm):
xx= -838.5 yy= -829.0 zz= 2106.5

D – H_3PTMTC

1	6	2.357042	0.052578	0.93268
2	6	1.413236	-0.46369	0.007866
3	6	1.879107	-1.43576	-0.91457
4	6	3.209434	-1.87212	-0.90114
5	6	4.121103	-1.34297	0.01552
6	6	3.690431	-0.37474	0.92556
7	6	0.004003	-0.00722	0.004752
8	6	-0.30341	1.442406	0.008133
9	6	0.308602	2.330633	-0.913
10	6	0.024873	3.70155	-0.89899
11	6	-0.88841	4.228239	0.01753
12	6	-1.51525	3.372029	0.925913
13	6	-1.22277	2.002706	0.931554
14	6	-1.09738	-0.99724	-0.00395
15	6	-1.12472	-2.08334	0.908826
16	6	-2.16247	-3.02319	0.889608
17	6	-3.21334	-2.9024	-0.02276
18	6	-3.21685	-1.83427	-0.92281
19	6	-2.17273	-0.90147	-0.92471
20	17	0.086048	-2.22327	2.152261
21	17	-2.19452	-4.35154	2.018476
22	6	-4.31144	-3.93901	-0.06486
23	17	-4.53575	-1.70943	-2.05638
24	17	-2.17691	0.330654	-2.15508
25	17	1.359504	1.721929	-2.16083
26	17	0.776013	4.786634	-2.03827
27	6	-1.16133	5.713705	0.05413
28	17	-2.64656	4.054241	2.063623
29	17	-1.94629	1.013116	2.16804
30	17	3.776646	-3.06216	-2.0421
31	6	5.545966	-1.84372	0.051066
32	17	4.845374	0.265408	2.063885
33	17	1.859083	1.166546	2.174596
34	17	0.828037	-2.04471	-2.16201

35	8	-5.34233	-3.60143	0.721209
36	8	-4.25266	-4.94782	-0.73279
37	1	-6.02454	-4.29576	0.661501
38	8	-2.18875	6.048779	-0.73737
39	8	-0.51906	6.494293	0.721576
40	1	-2.32786	7.012496	-0.6824
41	8	6.347532	-1.11409	-0.73602
42	8	5.904689	-2.79072	0.715752
43	1	7.253355	-1.47132	-0.68155

g value of the free electron [g_e]: 0.20023193D+01
relativistic mass correction [g_RMC]: -0.16525305D-03
diamagnetic correction to g tensor [g_DC]:
XX= 0.61205447D-04 YX=-0.34554580D-06 ZX= 0.19991741D-05
XY=-0.35576723D-06 YY= 0.58774461D-04 ZY= 0.36869991D-06
XZ=-0.41810602D-05 YZ=-0.64064979D-05 ZZ= 0.27893718D-04
orbital Zeeman and spin-orbit coupling contribution to g tensor [g_OZ/SOC]:
XX=-0.10583233D-02 YX=-0.30431673D-04 ZX= 0.36168479D-04
XY=-0.11365927D-04 YY=-0.10231297D-02 ZY=-0.23319459D-04
XZ=-0.13496772D-05 YZ= 0.19798457D-04 ZZ= 0.27942168D-02
g tensor [g = g_e + g_RMC + g_DC + g_OZ/SOC]:
XX= 0.20011569D+01 YX=-0.30777219D-04 ZX= 0.38167653D-04
XY=-0.11721695D-04 YY= 0.20011897D+01 ZY=-0.22950759D-04
XZ=-0.55307374D-05 YZ= 0.13391959D-04 ZZ= 0.20049762D+01
g shifts relative to the free electron (ppm):
xx= -1172.9 yy= -1119.2 zz= 2656.9

E – PTMTE

1	6	-2.11253	-0.93797	-0.98321
2	6	-1.06028	-1.04162	-0.03715
3	6	-1.09993	-2.14688	0.851584
4	6	-2.12836	-3.09476	0.7874
5	6	-3.15802	-2.96637	-0.14792
6	6	-3.14665	-1.8807	-1.02682
7	6	0.02888	-0.03978	0.021515
8	6	-0.29575	1.405665	0.049815
9	6	0.330357	2.322939	-0.83282
10	6	0.031253	3.690002	-0.79316
11	6	-0.91299	4.186477	0.10879
12	6	-1.55423	3.300491	0.977771
13	6	-1.24677	1.934635	0.959766
14	17	1.420694	1.755611	-2.06706
15	17	0.803425	4.81004	-1.88497
16	6	-1.20248	5.668958	0.174861
17	8	-0.58754	6.433699	0.889262
18	17	-2.72618	3.942221	2.09915

19	17	-1.99329	0.908417	2.152709
20	17	0.082001	-2.30173	2.12134
21	17	-2.17573	-4.44491	1.890808
22	6	-4.24601	-4.01237	-0.23701
23	8	-4.15373	-5.00991	-0.9223
24	17	-4.43651	-1.74502	-2.19341
25	17	-2.09619	0.319771	-2.18816
26	6	1.443042	-0.47989	0.0487
27	6	2.357792	0.024361	1.008655
28	6	3.696657	-0.38498	1.02222
29	6	4.164582	-1.3214	0.097308
30	6	3.280732	-1.83852	-0.85294
31	6	1.944518	-1.42203	-0.88596
32	17	1.814406	1.100141	2.26596
33	17	0.930292	-2.01562	-2.17146
34	17	3.891294	-2.98911	-2.01309
35	6	5.596855	-1.80257	0.151664
36	8	5.948737	-2.76933	0.795738
37	17	4.814359	0.239835	2.206583
38	8	-5.29033	-3.68883	0.525184
39	8	-2.20049	6.003743	-0.64233
40	8	6.39284	-1.03282	-0.58989
41	6	-6.40528	-4.61947	0.5267
42	6	-2.57435	7.406934	-0.66825
43	6	7.799254	-1.39383	-0.62162
44	1	-3.38519	7.470231	-1.39089
45	1	-2.90977	7.718363	0.322357
46	1	-1.72234	8.011273	-0.98379
47	1	8.267016	-0.65219	-1.26569
48	1	8.215031	-1.35285	0.386381
49	1	7.914207	-2.39715	-1.03507
50	1	-7.14037	-4.17902	1.19701
51	1	-6.80737	-4.71716	-0.483
52	1	-6.07474	-5.59191	0.895361

g value of the free electron [g_e]: 0.20023193D+01
relativistic mass correction [g_RMC]: -0.16528373D-03
diamagnetic correction to g tensor [g_DC]:
XX= 0.66138682D-04 YX= 0.76238730D-06 ZX= 0.98767409D-06
XY= 0.17263376D-06 YY= 0.64603611D-04 ZY=-0.24290312D-06
XZ=-0.45329369D-04 YZ=-0.43184936D-04 ZZ= 0.32735177D-04
orbital Zeeman and spin-orbit coupling contribution to g tensor [g_OZ/SOC]:
XX=-0.10219731D-02 YX=-0.23021950D-04 ZX=-0.64997789D-04
XY= 0.76130006D-05 YY=-0.10438627D-02 ZY=-0.11388088D-03
XZ=-0.62579568D-04 YZ=-0.43315998D-04 ZZ= 0.27381980D-02
g tensor [g = g_e + g_RMC + g_DC + g_OZ/SOC]:
XX= 0.20011982D+01 YX=-0.22259563D-04 ZX=-0.64010115D-04
XY= 0.77856344D-05 YY= 0.20011748D+01 ZY=-0.11412378D-03

XZ=-0.10790894D-03 YZ=-0.86500934D-04 ZZ= 0.20049250D+01
g shifts relative to the free electron (ppm):
xx= -1150.5 yy= -1119.8 zz= 2610.3

Full size reproduction of Figure 4