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Supporting Information

For

Electronegativity and Location of Anionic Ligands Drive Yttrium NMR for Molecular, Surface and Solid-State Structures

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1 Benchmarking of the Calculated Principal Components

1.1 $Y(OAr)_3$ and $Y(\kappa_2HOSi(OtBu)_3)(OSi(OtBu)_3)_3$

The computational protocol was validated by simulation of static solid state ^{89}Y NMR spectra (based on the calculated principal components). Good agreement was found for our DFT calculated spectra with the measured spectra of Delley *et al.*, suggesting that we are able to predict the principal components of the chemical shift tensor accurately.

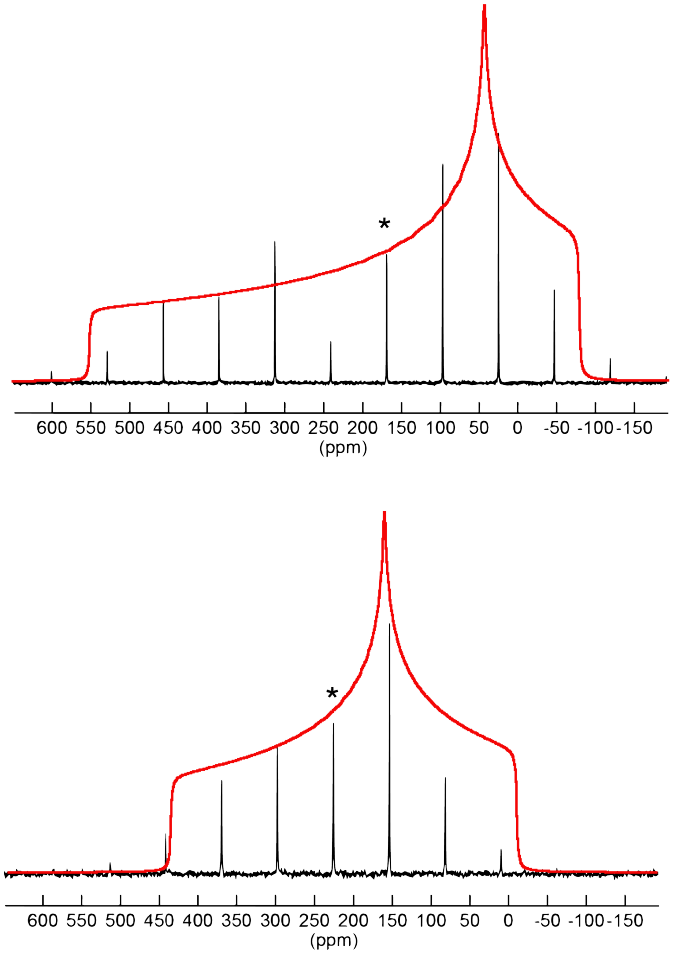


Figure S1: Solid state ^{89}Y NMR of $Y(OAr)_3$ (top, OAr = 2,6-Di-*tert*-butyl-4-methylphenoxy) and $Y(\kappa_2HOSi(OtBu)_3)(OSi(OtBu)_3)_3$ (bottom) measured by Delley *et al.* (in black). The isotropic peak is denoted with *. The DFT calculated static solid state ^{89}Y NMR spectra are depicted in red.

2 Comparison of Functionals for Reported Organoyttrium Compounds

When turning to the NCS analysis of large complexes (> 25 atoms) the method based on B3LYP proved to be unsuccessful. A protocol using a revPBE functional and a TZP basis set was successful and could be applied to the reported organoyttrium compounds. As exemplified below by the calculated isotropic chemical shieldings, both methods show the same trends, direct comparison of qualitative trends is thus legitimate and was performed throughout this study.

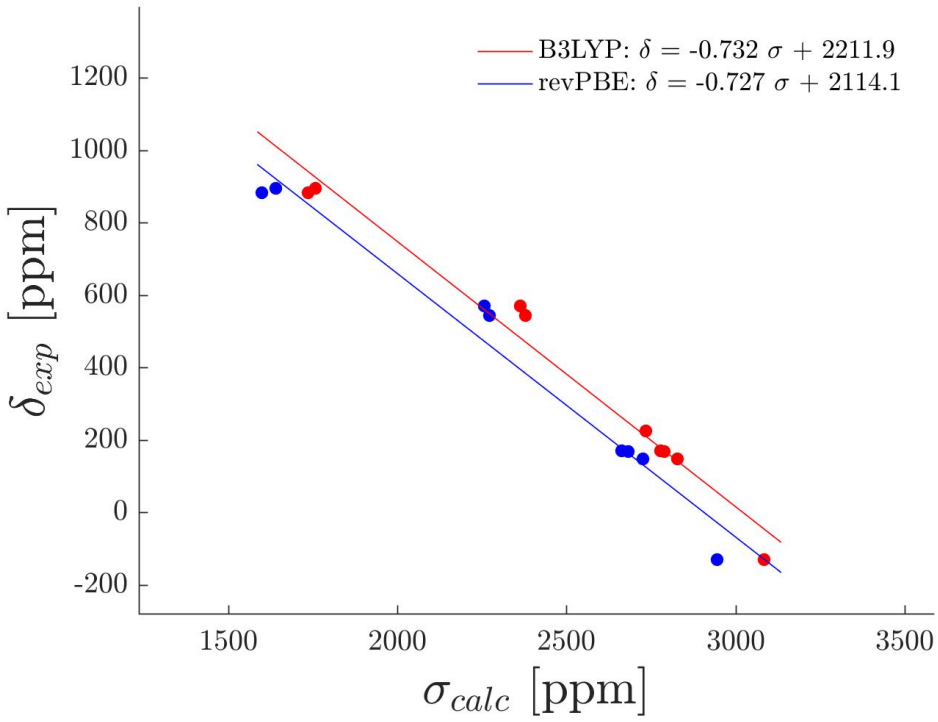


Figure S2: Correlation of the experimental observed chemical shift and the calculated chemical shielding. Both B3LYP and revPBE based calculations display excellent linear behaviour.

3 Optimized Structures of Investigated Yttrium Compounds

3.1 Organoyttrium Model Compounds

$Y(CH_3)_3$

Y	0.00090	-0.00030	0.35370
C	2.19691	-0.19883	-0.46098
H	2.39744	0.54389	-1.24959
H	2.38845	-1.19005	-0.90131
H	2.97144	-0.04329	0.31060
C	-1.27333	-1.80068	-0.45937
H	-2.27340	-1.48586	-0.79694
H	-1.42880	-2.60462	0.28127
H	-0.78096	-2.27386	-1.32400
C	-0.92704	2.00116	-0.45871
H	-0.15771	2.71709	-0.78839
H	-1.55648	2.53069	0.27773
H	-1.57426	1.80799	-1.32932

$Y(CH_3)_2(NH_2)$

Y	0.00012	0.04596	-0.24481
C	-2.03048	-1.03906	0.30993
H	-2.84980	-0.35952	0.59276
H	-1.88040	-1.71798	1.16638
H	-2.42354	-1.67271	-0.50478
C	1.90393	-1.25182	0.30380
H	2.85428	-0.89304	-0.12459
H	1.80059	-2.30758	0.00176
H	2.05439	-1.26556	1.39676
N	0.12511	2.11672	0.31797
H	-0.65513	2.72697	0.56155
H	0.97860	2.62528	0.54974

$Y(CH_3)(NH_2)_2$

Y	0.03882	0.00018	0.01918
C	-2.34524	0.03692	-0.02177
H	-2.80180	-0.71863	0.63997
H	-2.74806	-0.17400	-1.02799
H	-2.77815	1.00636	0.27550
N	1.06384	-1.90338	-0.02415
H	2.06936	-2.07176	-0.04137
H	0.61859	-2.82166	-0.04145
N	1.12835	1.86745	-0.02434
H	0.71318	2.79971	-0.04071
H	2.13879	2.00289	-0.04185

$Y(NH_2)_3$

Y	-0.00023	0.00028	0.00014

N	-2.07505	0.63492	-0.00016
H	-2.42343	1.59333	-0.00029
H	-2.89801	0.03263	-0.00049
N	1.58845	1.47792	-0.00016
H	2.59209	1.29718	-0.00040
H	1.48163	2.49211	-0.00037
N	0.48741	-2.11368	-0.00017
H	-0.16905	-2.89407	-0.00025
H	1.42013	-2.52604	-0.00038

YCl_3

Y	-0.00026	0.00450	0.11890
Cl	2.12347	1.21754	-0.09119
Cl	-2.12636	1.21189	-0.09125
Cl	0.00348	-2.43974	-0.09033

$Y(OH)_3$

Y	0.00039	-0.00007	0.00038
O	-0.81414	1.87134	-0.00050
H	-1.19806	2.75293	-0.00081
O	-1.21563	-1.63945	-0.00047
H	-1.78851	-2.41178	-0.00094
O	2.02819	-0.23213	-0.00066
H	2.98402	-0.33651	0.00008

$Y(OCH_3)_3$

Y	-0.00074	-0.00081	0.02766
O	0.33831	2.01722	-0.00157
O	-1.91966	-0.71446	0.00028
O	1.58155	-1.30077	-0.00162
C	0.59273	3.38890	-0.03592
H	-0.00859	3.88700	-0.81225
H	1.65319	3.59674	-0.24784
H	0.34614	3.86235	0.92706
C	2.64393	-2.20491	-0.03594
H	3.17429	-2.23068	0.92863
H	3.37798	-1.92912	-0.80897
H	2.29632	-3.22713	-0.25264
C	-3.23379	-1.18244	-0.03695
H	-3.92722	-0.40640	-0.39691
H	-3.57255	-1.49277	0.96366
H	-3.32948	-2.05380	-0.70334

$Y(N(CH_3)_2)_3$

Y	0.00027	-0.00033	0.00189
N	-0.52976	2.11992	0.00110
N	2.10213	-0.60146	0.00007

N	-1.57175	-1.51845	-0.00100
C	3.22578	0.30402	0.18206
H	2.87986	1.33520	0.33461
H	3.90576	0.31112	-0.68960
H	3.83902	0.03530	1.06169
C	2.58014	-1.96262	-0.18531
H	1.74286	-2.65744	-0.33468
H	3.15875	-2.32699	0.68331
H	3.23911	-2.05576	-1.06808
C	-1.35264	-2.94380	0.18823
H	-0.28796	-3.16111	0.34794
H	-1.68226	-3.53993	-0.68254
H	-1.89748	-3.33573	1.06664
C	-2.98849	-1.25028	-0.19294
H	-3.16940	-0.17802	-0.34740
H	-3.59756	-1.56403	0.67464
H	-3.39612	-1.77746	-1.07506
C	-1.87525	2.63958	0.18889
H	-2.59373	1.82414	0.34755
H	-2.22696	3.22240	-0.68220
H	-1.94526	3.30682	1.06749
C	0.40907	3.21446	-0.18862
H	1.42829	2.83668	-0.34547
H	0.44164	3.89615	0.68100
H	0.15505	3.83333	-1.06873

$Y(CH_3)_3$(thf)

Y	1.18928	0.00513	0.00715
C	1.93948	-0.42291	-2.21445
H	2.35858	-1.43667	-2.33029
H	2.73500	0.27716	-2.52156
H	1.14755	-0.33073	-2.97924
C	1.91837	2.12664	0.81903
H	1.10205	2.79372	1.15095
H	2.48462	2.69545	0.06249
H	2.58765	2.02021	1.68968
C	1.74358	-1.79037	1.47887
H	0.88979	-2.42829	1.77147
H	2.18921	-1.43350	2.42269
H	2.48337	-2.47250	1.02658
O	-1.19596	0.04279	-0.07066
C	-2.01167	-1.16634	-0.18633
C	-2.05177	1.22289	0.06332
C	-3.46988	0.72035	-0.20766
H	-1.70222	1.97459	-0.64842
H	-1.93375	1.60738	1.08137
C	-3.40470	-0.74027	0.26768
H	-3.69476	0.76533	-1.27903
H	-4.22028	1.31235	0.32337
H	-1.55106	-1.93747	0.43556

H	-1.99802	-1.48492	-1.23431
H	-4.18724	-1.36852	-0.16655
H	-3.48535	-0.79609	1.35901

***cis*-Y$(CH_3)_3$(thf)$_2$**

Y	-0.07239	1.27991	0.02722
O	1.43481	-0.78186	0.21803
O	-1.47087	-0.75216	-0.17432
C	-2.09064	2.52960	-0.42778
H	-1.87743	3.58035	-0.15685
H	-2.98164	2.25300	0.16416
H	-2.41647	2.56507	-1.48242
C	1.44267	2.00289	-1.69255
C	0.63058	1.97716	2.21091
H	2.48602	2.11002	-1.34711
H	1.13826	3.00209	-2.04847
H	1.48216	1.36762	-2.59570
H	1.62041	2.46611	2.20753
H	0.68699	1.18164	2.97533
H	-0.07518	2.72688	2.60774
C	2.64947	-0.64250	1.01240
C	1.69850	-1.59665	-0.95340
C	3.63882	-1.65084	0.42694
H	2.38775	-0.82476	2.05721
H	3.00813	0.38682	0.91398
C	3.21989	-1.69484	-1.05071
H	3.51089	-2.63530	0.89275
H	4.67724	-1.33918	0.57182
H	3.54641	-2.60180	-1.56819
H	3.61783	-0.82728	-1.58808
H	1.23917	-1.11180	-1.81821
H	1.23364	-2.58004	-0.80299
C	-2.63975	-0.81659	-1.04249
C	-1.60769	-1.70165	0.92275
C	-3.70840	-1.51630	-0.20877
H	-2.37163	-1.39845	-1.93369
H	-2.88630	0.20633	-1.32843
C	-2.87276	-2.50787	0.61645
H	-4.46723	-2.00280	-0.82841
H	-4.20876	-0.79392	0.44583
H	-2.62923	-3.39314	0.01750
H	-3.37520	-2.84356	1.52813
H	-1.70344	-1.13281	1.85506
H	-0.69486	-2.29955	0.96763

***trans*-Y$(CH_3)_3$(thf)$_2$**

Y	0.00365	-0.00573	0.04084
O	-2.41907	-0.00298	0.07533
O	2.42619	-0.00763	0.02774

C	-0.07822	-0.17800	-2.37650
H	-0.82242	0.50111	-2.83035
H	-0.34640	-1.19413	-2.71953
H	0.87556	0.05465	-2.88311
C	-0.04567	2.18413	1.09519
C	0.07463	-2.04571	1.35623
H	0.54630	-2.89399	0.82682
H	-0.92871	-2.40542	1.64660
H	0.62788	-1.93741	2.30664
H	-0.55121	2.95557	0.48558
H	0.95849	2.59337	1.30760
H	-0.56524	2.18224	2.07070
C	3.32134	-0.89385	0.75440
C	3.18987	0.97893	-0.72685
C	4.65059	0.76268	-0.32133
H	2.80469	1.97023	-0.47363
H	3.01822	0.78517	-1.79021
C	4.67349	-0.72459	0.06747
H	4.90599	1.38590	0.54324
H	5.34159	1.00826	-1.13281
H	5.50760	-0.98502	0.72562
H	4.72996	-1.35682	-0.82619
H	2.90213	-1.89931	0.70280
H	3.35399	-0.57256	1.80229
C	-3.18910	-0.99728	-0.66353
C	-3.30851	0.90866	0.77398
C	-4.64327	0.77274	0.04770
H	-2.85913	1.90141	0.73080
H	-3.38215	0.59172	1.82168
C	-4.65635	-0.72093	-0.31730
H	-4.64964	1.39202	-0.85665
H	-5.48922	1.07017	0.67436
H	-5.32454	-0.95590	-1.15070
H	-4.96739	-1.31997	0.54612
H	-2.84638	-1.98907	-0.35576
H	-2.97219	-0.85459	-1.72617

Y(CH$_3$)$_3$ - $\theta = 180^\circ$

Y	0.00006	-0.00016	-0.00023
C	-0.49591	2.31412	-0.00258
H	-1.26185	2.58792	-0.74895
H	0.37240	2.96482	-0.19678
H	-0.91050	2.64771	0.96608
C	2.25218	-0.72810	-0.00079
H	2.37613	-1.82287	-0.03327
H	2.80060	-0.38547	0.89506
H	2.82725	-0.32856	-0.85484
C	-1.75691	-1.58576	-0.00061
H	-2.76601	-1.14307	-0.03019
H	-1.73469	-2.23505	0.89292

H	-1.70187	-2.28061	-0.85729

3.2 Reported Organoyttrium Compounds

$Y(CH(SiMe_3)_2)_3$

Y	-0.00082	0.00087	-0.45593
C	1.30827	1.84793	0.28185
C	0.94747	-2.05574	0.27942
C	-2.25450	0.20764	0.28095
Si	1.43504	2.94138	-1.23317
Si	2.78479	1.75818	1.43773
H	0.48885	2.29258	0.88664
Si	-3.26213	-0.22532	-1.23676
Si	-2.91676	1.52677	1.44063
H	-2.22801	-0.72629	0.88292
Si	0.13407	-3.28728	1.43930
Si	1.82622	-2.71455	-1.23768
H	1.74403	-1.56675	0.88067
C	1.25154	-4.77574	1.85593
H	0.76632	-5.43945	2.58348
H	2.20297	-4.44714	2.29306
H	1.48833	-5.37918	0.97083
C	-0.27637	-2.45183	3.09807
H	-0.73878	-3.16721	3.79028
H	-0.97363	-1.61353	2.97875
H	0.62490	-2.06116	3.58675
C	-1.48759	-3.98883	0.73268
H	-2.23499	-3.20113	0.57738
H	-1.92249	-4.71719	1.42905
H	-1.33884	-4.50090	-0.22492
C	1.95067	-1.29718	-2.54479
H	0.98490	-1.01129	-2.99438
H	2.56018	-1.63347	-3.39371
H	2.44599	-0.39326	-2.16018
C	0.90970	-4.12482	-2.12130
H	-0.12241	-3.85941	-2.38004
H	0.87073	-5.03061	-1.50547
H	1.42586	-4.38464	-3.05431
C	3.61392	-3.27109	-0.92278
H	4.22113	-2.46036	-0.50248
H	4.09807	-3.60289	-1.85032
H	3.64287	-4.10577	-0.21259
C	-2.71675	3.28108	0.73199
H	-1.66199	3.53481	0.57027
H	-3.12635	4.02269	1.42965
H	-3.23985	3.40690	-0.22300
C	-4.76410	1.30030	1.85697
H	-5.40505	1.39204	0.97121
H	-5.09932	2.05377	2.58171
H	-4.95313	0.31315	2.29739

C	-1.98906	1.46557	3.10006
H	-0.91452	1.65145	2.98284
H	-2.10067	0.48927	3.58839
H	-2.37960	2.22281	3.79202
C	-4.63277	-1.50171	-0.92657
H	-4.23113	-2.43231	-0.50781
H	-5.16009	-1.75491	-1.85537
H	-5.37294	-1.11455	-0.21668
C	-2.09280	-1.03317	-2.54575
H	-1.55393	-1.91351	-2.16511
H	-1.36603	-0.33492	-2.99427
H	-2.68777	-1.39237	-3.39553
C	-4.03113	1.27088	-2.11973
H	-4.79882	1.75426	-1.50471
H	-4.51196	0.95183	-3.05319
H	-3.28855	2.03545	-2.37796
C	3.51176	3.47065	1.85781
H	3.91095	3.98135	0.97237
H	4.33229	3.38332	2.58236
H	2.75130	4.12677	2.29982
C	4.20377	0.71138	0.72216
H	4.57027	1.10276	-0.23379
H	3.89707	-0.32909	0.56074
H	5.05316	0.69602	1.41690
C	2.27172	0.97625	3.09400
H	1.47870	1.55421	3.58483
H	3.12255	0.93681	3.78634
H	1.90112	-0.04881	2.97103
C	0.14962	2.33800	-2.54349
H	0.38705	1.35845	-2.99185
H	-0.88269	2.31590	-2.16376
H	0.14012	3.03320	-3.39280
C	3.11490	2.86237	-2.11660
H	3.40212	1.83816	-2.38331
H	3.91799	3.27701	-1.49678
H	3.08143	3.44695	-3.04474
C	1.01389	4.76538	-0.91534
H	0.00787	4.88090	-0.49433
H	1.05568	5.35236	-1.84186
H	1.72039	5.21038	-0.20504

Y(N(SiMe$_3$)$_2$)$_3$

Y	0.00089	0.00151	-0.43051
N	2.06852	0.70581	0.04489
N	-0.43025	-2.14187	0.03581
N	-1.63834	1.44631	0.03331
Si	3.13530	0.11263	1.30130
Si	2.55478	1.88343	-1.13996
Si	-2.91779	1.25167	-1.12972
Si	-1.65120	2.69219	1.26516

Si	-1.54220	-2.76974	1.23561
Si	0.42202	-3.16553	-1.08478
C	-0.83889	-4.26208	2.18051
H	-1.53261	-4.56717	2.97480
H	0.12239	-4.02763	2.65326
H	-0.68683	-5.13384	1.53237
C	-1.93393	-1.43023	2.52052
H	-2.67330	-1.80364	3.24076
H	-2.34795	-0.52462	2.06229
H	-1.04110	-1.14435	3.09034
C	-3.19039	-3.32766	0.46814
H	-3.66332	-2.52302	-0.10751
H	-3.89862	-3.63425	1.24903
H	-3.05903	-4.17955	-0.20919
C	1.22018	-2.00581	-2.39447
H	0.48687	-1.44324	-2.99406
H	1.76299	-2.62540	-3.11957
H	1.96974	-1.31291	-1.98512
C	-0.68576	-4.36205	-2.05821
H	-1.51295	-3.84187	-2.55604
H	-1.12346	-5.12892	-1.40805
H	-0.10380	-4.88336	-2.82939
C	1.83478	-4.18081	-0.33151
H	2.52340	-3.55111	0.24275
H	2.41542	-4.68452	-1.11547
H	1.45721	-4.95470	0.34640
C	-1.27335	4.41574	0.55688
H	-0.31739	4.43302	0.01999
H	-1.21338	5.16041	1.36140
H	-2.04743	4.75076	-0.14360
C	-3.32184	2.81805	2.16357
H	-4.12653	3.16772	1.50518
H	-3.25045	3.53279	2.99382
H	-3.63095	1.85343	2.58330
C	-0.33694	2.31403	2.58010
H	0.66816	2.23338	2.15010
H	-0.55466	1.38043	3.11332
H	-0.31098	3.11672	3.32843
C	-4.54643	0.57385	-0.43537
H	-4.38924	-0.33198	0.16050
H	-5.24186	0.32540	-1.24783
H	-5.04338	1.30729	0.20933
C	-2.30006	-0.03763	-2.41834
H	-2.11145	-1.03751	-2.00066
H	-1.42223	0.29082	-2.99769
H	-3.09147	-0.17856	-3.16540
C	-3.32784	2.82069	-2.11725
H	-3.77065	3.59439	-1.47874
H	-4.05358	2.59913	-2.91055
H	-2.43711	3.25342	-2.58837

C	4.11860	1.42399	-2.11361
H	5.01403	1.45517	-1.48166
H	4.27996	2.12804	-2.94040
H	4.05263	0.41576	-2.53981
C	2.78850	3.64617	-0.48340
H	3.65855	3.71536	0.17916
H	1.91659	3.98711	0.08579
H	2.94718	4.35135	-1.30983
C	1.13866	1.97202	-2.44093
H	0.99266	1.04097	-3.01184
H	1.41757	2.72057	-3.19342
H	0.17298	2.31203	-2.03882
C	2.14507	-0.88784	2.57372
H	1.41332	-0.26341	3.10099
H	1.60853	-1.72723	2.11652
H	2.82255	-1.30258	3.33137
C	4.00695	1.51437	2.24429
H	3.29022	2.23891	2.64874
H	4.71493	2.06433	1.61229
H	4.57759	1.10551	3.08834
C	4.49708	-1.02521	0.61847
H	4.07791	-1.86029	0.04453
H	5.09123	-1.45275	1.43677
H	5.18774	-0.48903	-0.04240

Y(O-2,6-*t*-Bu$_2$C$_6$H$_3$)$_3$

Y	0.07018	-0.01048	0.00635
O	2.14720	-0.08412	0.00011
O	-1.21706	-1.63944	0.04516
O	-0.99793	1.76363	-0.07519
C	-1.90431	-2.76565	-0.23306
C	-1.73684	-3.42387	-1.48359
C	-2.80813	-3.28154	0.75145
C	-3.46958	-4.48001	0.47205
C	-2.43496	-4.62679	-1.68402
C	-3.28194	-5.16223	-0.72739
C	3.49165	-0.15149	0.02854
C	4.13788	-1.01033	0.96947
C	4.26032	0.63968	-0.87953
C	5.53920	-1.03966	0.97593
C	6.30303	-0.27172	0.10821
C	5.65722	0.55188	-0.80336
C	-1.60820	2.93430	0.19885
C	-1.44409	3.55287	1.46982
C	-2.42589	3.53757	-0.81068
C	-2.99934	4.78110	-0.53388
C	-2.05057	4.80501	1.66640
C	-2.80824	5.42509	0.68611
H	-4.15201	-4.90143	1.19979
H	-3.80351	-6.09664	-0.91543

H	-2.31328	-5.16135	-2.62112
H	6.05379	-1.68414	1.68206
H	7.38817	-0.31582	0.14083
H	6.26354	1.14814	-1.47801
H	-1.92734	5.31126	2.61898
H	-3.25915	6.39592	0.87146
H	-3.61354	5.26957	-1.28022
C	3.71758	1.61342	-1.96628
C	2.18649	1.72476	-2.12070
H	1.73164	0.76491	-2.39072
H	1.96669	2.42156	-2.93886
H	1.70562	2.12787	-1.22469
C	4.25597	1.17075	-3.35230
H	3.90408	0.16233	-3.60051
H	5.34877	1.15780	-3.39120
H	3.90457	1.85597	-4.13402
C	4.22476	3.04543	-1.65379
H	3.84451	3.38874	-0.68482
H	3.88022	3.74941	-2.42197
H	5.31691	3.09933	-1.61877
C	3.45309	-1.94215	2.01256
C	1.91079	-1.94651	2.06017
H	1.50795	-0.96228	2.33040
H	1.58367	-2.64306	2.84098
H	1.46660	-2.29429	1.12240
C	3.87407	-3.40758	1.72566
H	3.53989	-3.71957	0.72892
H	3.42507	-4.08585	2.46211
H	4.95853	-3.54221	1.76777
C	3.92606	-1.54372	3.43466
H	3.63331	-0.51274	3.66723
H	5.01191	-1.61090	3.54584
H	3.47397	-2.20406	4.18560
C	-0.86951	-2.95526	-2.68765
C	-1.78503	-2.79104	-3.93003
H	-2.30683	-3.71791	-4.18179
H	-1.19422	-2.49372	-4.80571
H	-2.54545	-2.02139	-3.75270
C	0.21607	-4.02149	-2.98363
H	-0.22229	-4.99713	-3.21038
H	0.88004	-4.14968	-2.12040
H	0.82799	-3.72251	-3.84382
C	-0.11977	-1.61119	-2.54711
H	-0.81437	-0.78057	-2.35479
H	0.38060	-1.37763	-3.49398
H	0.68280	-1.67542	-1.79924
C	-3.07546	-2.54618	2.08699
C	-4.12494	-3.27558	2.95554
H	-5.09331	-3.35925	2.45011
H	-4.28409	-2.70573	3.87844

H	-3.79784	-4.28084	3.24405
C	-1.78674	-2.46759	2.93940
H	-1.42988	-3.47384	3.18931
H	-1.98314	-1.93739	3.88025
H	-0.98087	-1.95293	2.41512
C	-3.64082	-1.12981	1.81734
H	-2.96943	-0.52519	1.20561
H	-3.81648	-0.60388	2.76497
H	-4.59995	-1.19576	1.29049
C	-0.67282	2.99089	2.69866
C	-0.03310	1.59063	2.55873
H	-0.79036	0.82621	2.32839
H	0.41027	1.29978	3.51813
H	0.79620	1.59798	1.83774
C	-1.65233	2.88147	3.89733
H	-2.46777	2.18453	3.67078
H	-2.10296	3.84452	4.15038
H	-1.12728	2.51635	4.78919
C	0.48341	3.95563	3.06517
H	0.11749	4.96091	3.29158
H	1.19660	4.04064	2.23699
H	1.02508	3.59123	3.94730
C	-2.69676	2.84739	-2.16943
C	-3.64723	3.67310	-3.06542
H	-4.62592	3.82762	-2.59776
H	-3.81393	3.13220	-4.00416
H	-3.22894	4.65276	-3.32256
C	-3.38759	1.47883	-1.94918
H	-4.36182	1.61634	-1.46578
H	-2.79838	0.81181	-1.31781
H	-3.56031	0.98159	-2.91267
C	-1.38482	2.67493	-2.97078
H	-0.93455	3.65110	-3.18628
H	-1.58603	2.17896	-3.92921
H	-0.64716	2.08591	-2.42538

Y(OAr)$_3$

Y	0.00190	0.01658	0.31922
O	-1.84502	0.84709	-0.10544
O	1.65359	1.24502	0.07958
O	0.09917	-2.03997	0.06736
C	-3.01121	1.52588	-0.07006
C	-3.84531	1.53288	-1.23443
C	-5.03967	2.25144	-1.18190
H	-5.68649	2.27573	-2.05174
C	-5.45560	2.95443	-0.04643
C	-4.63079	2.91549	1.06909
H	-4.95390	3.45505	1.95503
C	-3.41071	2.21732	1.10405
C	-3.45796	0.77177	-2.52529

C	-2.13811	1.33004	-3.10866
H	-1.85917	0.77864	-4.01557
H	-1.31329	1.26059	-2.39865
H	-2.25470	2.38638	-3.37868
C	-3.33392	-0.74548	-2.24323
H	-4.29463	-1.15068	-1.90377
H	-2.59037	-0.96508	-1.47628
H	-3.04936	-1.27928	-3.15887
C	-4.52138	0.92178	-3.63598
H	-5.49497	0.52041	-3.33328
H	-4.19600	0.36164	-4.52009
H	-4.65810	1.96537	-3.94109
C	-6.75812	3.72187	-0.04395
H	-6.93900	4.19763	0.92585
H	-7.61407	3.06815	-0.25639
H	-6.76413	4.51241	-0.80574
C	-2.65026	2.29158	2.45934
C	-1.30433	1.53839	2.56013
H	-0.89802	1.65972	3.57116
H	-0.55710	1.96635	1.87723
H	-1.44281	0.45520	2.41706
C	2.87041	1.83223	0.08748
C	3.80787	1.54706	1.11549
C	5.05650	2.19131	1.05703
H	5.78841	1.98994	1.83423
C	5.41173	3.08108	0.05272
C	4.46132	3.34999	-0.93712
H	4.73290	4.05307	-1.71618
C	3.19710	2.76075	-0.95342
C	3.61024	0.60906	2.34113
C	2.19145	3.12769	-2.07132
C	2.76554	4.16720	-3.06032
H	3.02006	5.11147	-2.56625
H	2.01085	4.38916	-3.82352
H	3.65737	3.79777	-3.57888
C	0.91693	3.76295	-1.46326
H	0.41671	3.09299	-0.76294
H	0.20479	4.02212	-2.25661
H	1.17142	4.68445	-0.92597
C	1.83766	1.87974	-2.91533
H	2.73473	1.48091	-3.40366
H	1.11318	2.13903	-3.69704
H	1.40983	1.07977	-2.30874
C	0.12377	-3.38165	-0.10512
C	0.85308	-3.94260	-1.19509
C	0.85613	-5.33543	-1.33166
H	1.39986	-5.78814	-2.15279
C	0.18619	-6.18626	-0.45316
C	-0.52520	-5.60649	0.59595
H	-1.05394	-6.26935	1.27115

C	-0.58432	-4.22296	0.80321
C	1.62409	-3.06844	-2.21412
C	0.65851	-2.11160	-2.95389
H	-0.07183	-2.68126	-3.54006
H	0.09063	-1.47902	-2.26769
C	0.25018	-7.68774	-0.61958
H	-0.63289	-8.17676	-0.19316
H	1.12993	-8.11528	-0.11826
H	0.31270	-7.97321	-1.67599
C	-1.41301	-3.65942	1.98415
C	-0.50895	-2.86974	2.96124
H	0.24564	-3.52906	3.40574
H	-1.10507	-2.44134	3.77754
H	0.03132	-2.06061	2.46385
C	-2.07528	-4.77316	2.82613
H	-2.77820	-5.37138	2.23661
H	-2.64143	-4.31532	3.64574
H	-1.33746	-5.44886	3.27247
C	-2.56729	-2.77025	1.46149
H	-2.21754	-1.94737	0.83528
H	-3.13702	-2.34805	2.30000
H	-3.25928	-3.36354	0.85309
C	6.77304	3.73760	0.01963
H	7.34532	3.51683	0.92709
H	6.69399	4.82878	-0.06571
H	7.36867	3.39306	-0.83637
C	3.71932	1.45190	3.63828
H	2.93547	2.21809	3.67084
H	4.68262	1.96341	3.71388
H	3.61023	0.81252	4.52376
C	2.27485	-0.16018	2.44180
H	2.14540	-0.86269	1.60957
H	1.42058	0.52456	2.53764
H	2.28101	-0.76870	3.35360
C	4.71561	-0.47951	2.34008
H	4.65197	-1.09624	1.43627
H	4.60501	-1.13781	3.21111
H	5.71970	-0.04902	2.37757
C	-3.54788	1.70304	3.57870
H	-3.04383	1.76847	4.55153
H	-3.77542	0.64895	3.38058
H	-4.49914	2.23483	3.66202
C	-2.32425	3.77258	2.78290
H	-1.80395	3.85168	3.74608
H	-3.22751	4.38530	2.84335
H	-1.68065	4.20643	2.00891
C	2.31229	-3.91070	-3.31226
H	1.59208	-4.49282	-3.89767
H	3.05762	-4.59906	-2.89901
H	2.83351	-3.23938	-4.00465

C	2.75166	-2.27870	-1.50643
H	2.37263	-1.62552	-0.71855
H	3.29654	-1.65652	-2.22707
H	3.46872	-2.96922	-1.04686
H	1.21226	-1.46062	-3.64163

Y(κ_2HOSi(OtBu)$_3$)(OSi(OtBu)$_3$)$_3$

Y	0.14764	0.04359	-0.05326
O	-0.92269	1.07382	-1.60275
O	0.01523	-2.01159	-0.47353
O	-1.48690	1.29067	1.22566
O	0.06679	-0.03067	2.51565
O	2.13822	0.70736	-0.23813
Si	-0.46478	-3.55557	-0.36332
Si	-2.27833	1.80136	-2.07184
Si	3.74742	0.89304	-0.27896
O	0.43160	-4.47172	0.69355
O	-2.01239	-3.50416	0.22995
O	-0.37845	-4.37307	-1.80625
O	-2.06656	3.30075	-2.74280
O	-3.23986	0.97901	-3.13285
O	-3.22031	1.94008	-0.65915
O	4.40038	-0.40260	0.52675
O	4.28345	2.24386	0.52170
O	4.34669	1.02247	-1.82216
C	1.64490	-5.23606	0.51012
C	2.19803	-5.48339	1.92011
H	2.46235	-4.53944	2.40606
H	3.09424	-6.11302	1.87886
H	1.44822	-5.98994	2.53765
C	2.66035	-4.45267	-0.33414
H	2.87886	-3.48006	0.11775
H	2.27374	-4.28628	-1.34391
H	3.60009	-5.01186	-0.41602
C	1.30365	-6.57735	-0.15679
H	0.60176	-7.14456	0.46525
H	2.20866	-7.18336	-0.28552
H	0.84678	-6.41150	-1.13486
C	-2.84467	-4.47529	0.88424
C	-2.70941	-5.86165	0.23685
H	-2.95723	-5.81648	-0.82842
H	-3.38851	-6.57526	0.71825
H	-1.68843	-6.23977	0.33496
C	-2.45574	-4.53155	2.37008
H	-1.41845	-4.86105	2.47625
H	-3.10490	-5.22265	2.92159
H	-2.54892	-3.53522	2.81837
C	-4.28118	-3.95815	0.72517
H	-4.36858	-2.95075	1.14599
H	-4.99480	-4.61477	1.23667

H	-4.55404	-3.90662	-0.33429
C	-0.77690	-4.02761	-3.14344
C	0.24887	-3.05316	-3.74049
C	-0.77723	-5.34825	-3.92589
H	-1.05327	-5.18272	-4.97374
H	-1.49074	-6.05286	-3.48522
H	0.21715	-5.80673	-3.89832
C	-2.18179	-3.40995	-3.14931
C	-3.17390	0.81144	-4.56803
C	-3.68960	2.08139	-5.26108
H	-4.72175	2.28995	-4.95758
H	-3.67661	1.95265	-6.34996
H	-3.07265	2.94395	-4.99972
C	-1.73525	0.49939	-5.00195
H	-1.07036	1.34310	-4.78950
H	-1.69523	0.30070	-6.07936
H	-1.35431	-0.37849	-4.47192
C	-4.10123	-0.36894	-4.88189
H	-3.76500	-1.26983	-4.36145
H	-4.11997	-0.57181	-5.95891
H	-5.12336	-0.14592	-4.55665
C	-4.66023	2.12779	-0.52553
C	-4.87726	2.66395	0.89359
H	-4.47377	1.96464	1.63391
H	-5.94580	2.79142	1.09869
H	-4.38440	3.63336	1.02437
C	-5.17706	3.14725	-1.54808
H	-4.65094	4.10127	-1.44431
H	-6.24741	3.32184	-1.38890
H	-5.03590	2.78556	-2.56849
C	-5.34780	0.76706	-0.69737
H	-4.96600	0.04999	0.03850
H	-5.15396	0.36890	-1.69562
H	-6.43099	0.86191	-0.55567
C	-1.10106	4.34679	-2.53043
C	0.21231	3.95987	-3.22294
H	0.96144	4.75272	-3.11299
H	0.04042	3.79749	-4.29297
H	0.61374	3.03819	-2.79342
C	-0.88190	4.58035	-1.02957
H	-0.45592	3.68828	-0.56057
H	-1.83127	4.81489	-0.53587
H	-0.19087	5.41481	-0.86425
C	-1.70314	5.60033	-3.17884
H	-2.65574	5.85805	-2.70345
H	-1.88965	5.42571	-4.24370
H	-1.02316	6.45445	-3.08236
C	5.71546	-0.64103	1.06606
C	5.82993	-2.16348	1.22128
H	5.74345	-2.65685	0.24735

H	5.02992	-2.54259	1.86572
H	6.79345	-2.43899	1.66585
C	6.81449	-0.12621	0.12428
H	6.74470	0.95698	-0.00610
H	6.73538	-0.59558	-0.86123
H	7.80343	-0.35854	0.53677
C	5.81888	0.04458	2.43712
H	5.04535	-0.33987	3.11099
H	5.67814	1.12334	2.33135
H	6.79738	-0.14331	2.89538
C	4.41886	3.62116	0.12711
C	5.71737	3.78922	-0.67670
H	6.57942	3.48537	-0.07207
H	5.85996	4.83577	-0.97211
H	5.68922	3.16867	-1.57602
C	3.20789	4.07387	-0.70012
H	3.14763	3.51375	-1.63756
H	3.28495	5.14065	-0.94255
H	2.28011	3.91149	-0.14205
C	4.49732	4.41893	1.43581
H	5.33861	4.06967	2.04408
H	3.57837	4.29035	2.01777
H	4.63605	5.48768	1.23505
C	4.06827	0.28082	-3.02620
C	2.79625	0.84532	-3.67455
H	1.93634	0.72925	-3.00893
H	2.92228	1.91257	-3.88819
H	2.57706	0.33037	-4.61758
C	5.27853	0.51485	-3.94072
H	5.40966	1.58574	-4.13045
H	5.14661	0.00634	-4.90279
H	6.19268	0.13707	-3.47049
C	3.90945	-1.21796	-2.73100
H	3.74410	-1.77266	-3.66193
H	4.80801	-1.61582	-2.24911
H	3.05723	-1.40595	-2.07045
Si	-1.29800	0.89540	2.83187
O	-2.51255	-0.01943	3.39344
O	-1.02036	2.16037	3.82495
C	-3.61174	-0.02016	4.34330
C	-3.17402	-0.82341	5.57356
H	-2.83987	-1.82377	5.28280
H	-4.01201	-0.92929	6.27149
H	-2.35650	-0.32105	6.10055
C	-4.77120	-0.72474	3.62993
H	-4.47347	-1.73086	3.31995
H	-5.07450	-0.16740	2.73788
H	-5.63734	-0.80741	4.29581
C	-4.00725	1.40309	4.75149
H	-4.85009	1.36194	5.45031

H	-3.17654	1.91695	5.24096
H	-4.32066	1.99272	3.88398
C	-0.67331	3.56487	3.65151
C	-0.36734	4.07804	5.06226
H	-0.11069	5.14256	5.03475
H	0.47567	3.53136	5.49721
H	-1.23596	3.94812	5.71618
C	-1.88141	4.29689	3.05616
H	-1.67115	5.36825	2.96463
H	-2.76188	4.17353	3.69484
H	-2.11373	3.91239	2.05856
C	0.55234	3.70760	2.74385
H	0.35154	3.31035	1.74459
H	1.41573	3.18165	3.15910
H	0.81664	4.76534	2.63575
C	1.04366	-0.64858	3.44436
H	-2.20016	-2.46353	-2.59917
H	-2.90427	-4.08916	-2.68563
H	-2.50501	-3.21572	-4.17832
H	1.24791	-3.50315	-3.73488
H	0.28561	-2.13103	-3.15406
H	-0.00861	-2.80169	-4.77640
C	1.97601	0.44825	3.96245
H	2.48281	0.94752	3.13103
H	2.74168	0.00628	4.60989
H	1.42326	1.19032	4.54556
C	0.29235	-1.32928	4.58874
H	-0.23728	-0.60140	5.21128
H	1.00622	-1.85642	5.23094
H	-0.42789	-2.05697	4.20453
C	1.81605	-1.67586	2.62062
H	2.39521	-1.19897	1.82342
H	1.14771	-2.42484	2.18701
H	2.53008	-2.19278	3.27194
H	-2.28903	1.55737	0.68414

$Y(CH_2(SiMe_3))_3(thf)_2$

Y	0.14696	0.07429	-0.24954
O	1.00078	2.11729	-1.29867
O	-0.51270	-1.99712	0.83981
C	-0.52034	-3.27785	0.13301
C	-0.86943	-2.19999	2.24216
C	-1.13010	-4.28080	1.11188
H	0.51444	-3.52153	-0.11972
H	-1.10069	-3.15201	-0.78294
C	-0.72275	-3.70071	2.47455
H	-1.90005	-1.85868	2.38199
H	-0.20204	-1.58499	2.84655
H	-0.75372	-5.29394	0.94372
H	-2.22130	-4.30021	1.01357

H	-1.35148	-4.05137	3.29814
H	0.31899	-3.95160	2.70295
C	2.40328	2.50018	-1.18365
C	0.24323	3.18260	-1.94908
C	1.29625	4.10805	-2.55361
H	-0.35631	3.68854	-1.18545
H	-0.42198	2.71825	-2.67766
C	2.45168	3.98268	-1.54925
H	0.92781	5.13208	-2.66347
H	1.60487	3.74688	-3.54154
H	2.26041	4.60309	-0.66612
H	3.42146	4.27090	-1.96504
H	2.97758	1.88208	-1.88125
H	2.73122	2.28457	-0.16489
C	2.04487	-1.09170	-1.22672
C	-1.82602	0.41520	-1.62893
C	0.38253	1.18189	1.90594
Si	3.59241	-1.63055	-0.33287
H	2.34684	-0.45668	-2.08130
H	1.59056	-1.98677	-1.69530
Si	-3.29753	-0.68019	-1.96563
H	-1.40700	0.68366	-2.61830
H	-2.21412	1.36425	-1.20611
Si	-0.95044	2.19877	2.72478
H	0.73884	0.42035	2.62447
H	1.25385	1.84875	1.75364
C	-2.50810	1.15649	3.07795
H	-2.92515	0.72540	2.15827
H	-3.29528	1.76581	3.54004
H	-2.29372	0.32934	3.76718
C	-0.42283	2.97555	4.38628
H	-0.13074	2.20306	5.10930
H	-1.23064	3.56485	4.84030
H	0.44036	3.64110	4.25705
C	-1.48230	3.63299	1.58627
H	-0.62685	4.26877	1.32158
H	-2.23090	4.27545	2.06671
H	-1.92276	3.25678	0.65371
C	-2.81847	-2.10505	-3.13924
H	-2.48546	-1.71127	-4.10824
H	-3.67078	-2.76925	-3.33062
H	-2.00015	-2.72309	-2.74823
C	-4.74390	0.24094	-2.80407
H	-4.43375	0.67415	-3.76367
H	-5.10452	1.06590	-2.17593
H	-5.59773	-0.42127	-3.00017
C	-4.00558	-1.42971	-0.36108
H	-3.26274	-2.04745	0.15796
H	-4.88392	-2.05705	-0.55988
H	-4.31755	-0.64169	0.33696

C	3.19755	-2.85479	1.07794
H	2.50742	-2.41707	1.81052
H	4.11061	-3.13963	1.61607
H	2.74479	-3.78120	0.70028
C	4.86657	-2.49800	-1.45881
H	4.44127	-3.40153	-1.91444
H	5.76839	-2.79713	-0.90812
H	5.18211	-1.84028	-2.27896
C	4.48940	-0.15024	0.46799
H	3.85265	0.35935	1.20296
H	4.79835	0.59154	-0.27995
H	5.39695	-0.47690	0.99146

$Y(N(SiMe_3)_2)_3(OPPh_3)$

Y	-1.01023	-0.00028	-0.00061
N	-1.66868	-2.08114	-0.68004
N	-1.67036	1.62877	-1.46227
N	-1.67210	0.45093	2.14055
Si	-2.84999	-2.38004	-1.95033
Si	-0.94395	-3.47845	0.08442
Si	-0.94748	1.81120	2.96911
Si	-2.85418	-0.49940	3.03362
Si	-2.85089	2.87861	-1.08506
Si	-0.94551	1.66643	-3.05438
C	-3.90576	3.45406	-2.56615
H	-4.64077	4.18332	-2.19962
H	-4.46414	2.62865	-3.02207
H	-3.32890	3.94779	-3.35633
C	-4.12854	2.27881	0.18233
H	-4.78193	3.11221	0.47310
H	-3.67438	1.87463	1.09076
H	-4.76495	1.49898	-0.25319
C	-2.03886	4.47041	-0.42359
H	-1.48535	4.31084	0.50711
H	-2.80118	5.23565	-0.22545
H	-1.33787	4.88656	-1.15756
C	0.44544	0.36752	-3.18737
H	1.34576	0.68790	-2.65594
H	0.71186	0.24393	-4.24524
H	0.15307	-0.62305	-2.81677
C	-0.12057	3.33178	-3.47627
H	0.63270	3.60714	-2.72870
H	-0.84524	4.15222	-3.53573
H	0.38416	3.27122	-4.44978
C	-2.11229	1.27780	-4.50880
H	-2.66083	0.34145	-4.36345
H	-1.51864	1.17253	-5.42719
H	-2.84862	2.06725	-4.68507
C	-2.04405	-1.86757	4.08357
H	-1.49213	-2.59562	3.48080

H	-2.80727	-2.41969	4.64808
H	-1.34205	-1.44052	4.81021
C	-3.91040	0.49741	4.26965
H	-3.33428	0.93689	5.09176
H	-4.64557	-0.18388	4.71882
H	-4.46857	1.30370	3.78043
C	-4.12996	-1.29867	1.87967
H	-3.67444	-1.88566	1.07789
H	-4.76487	-0.53231	1.41878
H	-4.78503	-1.96532	2.45627
C	-2.11493	3.26491	3.35885
C	0.44366	2.57607	1.91118
H	0.15191	2.75032	0.86782
H	1.34454	1.95648	1.92383
H	0.70901	3.55424	2.33323
C	-0.12276	1.34494	4.62266
H	-0.84741	0.98570	5.36274
H	0.38076	2.21909	5.05689
H	0.63151	0.56069	4.48813
C	-0.11828	-4.67657	-1.14625
H	-0.84281	-5.13770	-1.82751
H	0.38578	-5.48973	-0.60689
H	0.63560	-4.16701	-1.75785
C	-2.11149	-4.54331	1.14806
H	-2.84644	-5.09227	0.55222
H	-2.66169	-3.94869	1.88460
H	-1.51824	-5.28486	1.70042
C	0.44663	-2.94442	1.27630
C	-4.12778	-0.98269	-2.06502
H	-4.76256	-0.96776	-1.17077
H	-3.67393	0.00591	-2.17257
H	-4.78277	-1.14961	-2.93053
C	-3.90488	-3.95015	-1.70667
C	-2.03968	-2.60374	-3.66037
H	-1.48647	-1.71809	-3.98846
H	-2.80306	-2.81459	-4.42118
H	-1.33891	-3.44756	-3.65485
H	-2.66595	3.60405	2.47561
H	-1.52162	4.11466	3.72328
H	-2.84915	3.02404	4.13300
O	1.31222	-0.00042	-0.00003
P	2.84909	0.00002	0.00064
C	3.53088	-1.54868	-0.67292
C	3.52999	0.19154	1.67902
C	3.53038	1.35800	-1.00388
C	2.97214	2.64179	-0.88043
C	3.50143	3.70611	-1.60907
C	4.62205	1.15767	-1.86333
C	4.58741	3.50075	-2.46393
C	5.14625	2.22803	-2.58998

H	2.12574	2.80708	-0.22260
H	3.06107	4.69416	-1.51248
H	4.99480	4.33173	-3.03299
H	5.98755	2.06400	-3.25725
H	5.05962	0.17056	-1.97131
C	4.61773	1.04074	1.93638
C	5.14116	1.13617	3.22691
C	4.58538	0.38738	4.26534
C	3.50329	-0.46029	4.01471
C	2.97478	-0.56050	2.72845
C	4.61978	-2.19488	-0.06704
H	-4.46375	-3.93128	-0.76420
H	-3.32812	-4.88143	-1.73792
H	-4.63961	-3.99818	-2.52171
H	2.13114	-1.21626	2.54229
H	5.05277	1.63071	1.13628
H	5.97937	1.79976	3.41928
H	4.99195	0.46597	5.26975
H	3.06508	-1.04035	4.82156
C	2.97514	-2.08193	-1.84844
C	3.50415	-3.24565	-2.40500
C	5.14377	-3.35985	-0.62992
C	4.58742	-3.88540	-1.79704
H	0.15577	-2.12594	1.94677
H	1.34862	-2.64833	0.73358
H	0.70993	-3.79816	1.91443
H	4.99444	-4.79423	-2.23144
H	3.06560	-3.65489	-3.31036
H	5.05505	-1.79614	0.84347
H	5.98279	-3.85748	-0.15204
H	2.13059	-1.59350	-2.32243

$Y(OAr)_3(OPMe_2Ph)$

Y	0.30876	0.27028	-0.02364
O	2.40128	0.09902	0.13295
O	-0.78137	-1.14892	1.12111
O	-0.49312	2.23512	-0.08349
C	-1.55359	-2.11060	1.66998
C	-1.30443	-3.49664	1.43254
C	-2.67101	-1.73268	2.49735
C	-3.53610	-2.72767	2.95389
C	-2.22524	-4.42991	1.94408
C	-3.34913	-4.08512	2.67937
C	3.71467	-0.16059	0.01035
C	4.43000	-0.83352	1.05461
C	4.41584	0.21409	-1.18117
C	5.74220	-1.24870	0.79265
C	6.40503	-1.00817	-0.40751
C	5.72637	-0.25128	-1.35643
C	-1.06749	3.43676	0.13875

C	-0.69806	4.25300	1.25080
C	-2.07358	3.91820	-0.77041
C	-2.74030	5.10784	-0.47064
C	-1.40997	5.44588	1.46336
C	-2.44633	5.88332	0.65151
H	-4.39007	-2.45072	3.56111
H	-2.04908	-5.48646	1.76421
H	6.28369	-1.78521	1.56685
H	6.25191	-0.00655	-2.27571
H	-1.13390	6.07407	2.30522
H	-3.51654	5.46774	-1.13592
C	3.89561	1.13031	-2.32810
C	2.50307	1.76315	-2.14378
H	1.70416	1.02178	-2.23805
H	2.33723	2.49465	-2.94501
H	2.40461	2.29181	-1.19333
C	3.85530	0.33105	-3.65473
H	3.17691	-0.52709	-3.56426
H	4.83901	-0.05707	-3.93581
H	3.49921	0.96600	-4.47735
C	4.87483	2.32588	-2.48708
H	4.89727	2.92727	-1.57097
H	4.55212	2.97512	-3.31107
H	5.89919	2.00741	-2.69768
C	3.93841	-1.12481	2.50499
C	2.51747	-0.65398	2.86880
H	2.39074	0.41218	2.68307
H	2.35605	-0.82878	3.94050
H	1.73477	-1.19861	2.33712
C	4.00418	-2.64568	2.79341
H	3.36090	-3.20368	2.10501
H	3.66305	-2.85056	3.81638
H	5.01826	-3.04582	2.69806
C	4.88811	-0.38724	3.48881
H	4.84038	0.69687	3.33229
H	5.93178	-0.69273	3.37148
H	4.59394	-0.59367	4.52573
C	-0.08551	-4.14109	0.70798
C	-0.57771	-5.06961	-0.43379
H	-1.21428	-5.88324	-0.07497
H	0.28085	-5.52862	-0.94187
H	-1.15600	-4.50570	-1.17497
C	0.69854	-4.99290	1.74117
H	0.07676	-5.77347	2.18954
H	1.07789	-4.36276	2.55299
H	1.55642	-5.48197	1.26149
C	0.93403	-3.17954	0.07288
H	0.48568	-2.57084	-0.71488
H	1.73920	-3.76858	-0.38571
H	1.39945	-2.51794	0.80247

C	-2.92038	-0.26944	2.93584
C	-4.11430	-0.13356	3.90875
H	-5.06385	-0.42756	3.44674
H	-4.20932	0.91664	4.20786
H	-3.97628	-0.72501	4.82064
C	-1.68147	0.25372	3.70056
H	-1.53672	-0.31722	4.62558
H	-1.81618	1.30768	3.97250
H	-0.76963	0.16083	3.10934
C	-3.25135	0.62999	1.72466
H	-2.45301	0.63985	0.98542
H	-3.41690	1.66575	2.04466
H	-4.16566	0.27963	1.22967
C	0.48050	4.02973	2.24005
C	1.21233	2.68265	2.14189
H	0.53754	1.84541	2.35419
H	1.99827	2.65036	2.90614
H	1.69951	2.53762	1.17606
C	-0.01460	4.14048	3.70620
H	-0.78396	3.38914	3.91543
H	-0.43530	5.12177	3.94165
H	0.82075	3.97020	4.39691
C	1.54320	5.13003	1.98247
H	1.12800	6.13461	2.10881
H	1.93529	5.05799	0.96112
H	2.38494	5.02184	2.67887
C	-2.39610	3.20708	-2.10677
C	-3.43362	3.97636	-2.95665
H	-4.40620	4.05309	-2.45790
H	-3.59265	3.43779	-3.89887
H	-3.09498	4.98694	-3.20933
C	-2.99388	1.80239	-1.87249
H	-3.92127	1.87273	-1.29282
H	-2.31031	1.15255	-1.32921
H	-3.23851	1.32176	-2.83022
C	-1.10804	3.13310	-2.96046
H	-0.72046	4.14196	-3.14488
H	-1.31856	2.67960	-3.93825
H	-0.32619	2.55749	-2.46498
C	-3.21889	7.14558	0.95824
H	-3.44831	7.71100	0.04682
H	-2.65612	7.80604	1.62750
H	-4.17781	6.92782	1.44949
C	7.79887	-1.53514	-0.66061
H	7.78411	-2.57186	-1.02610
H	8.40478	-1.52744	0.25318
H	8.32363	-0.93549	-1.41316
C	-4.31163	-5.12769	3.20109
H	-4.04776	-6.12837	2.84189
H	-5.34355	-4.92407	2.88607

H	-4.31694	-5.16341	4.29874
O	-0.23701	-0.57898	-2.06964
P	-0.70569	-1.33797	-3.31749
C	0.46261	-2.66219	-3.77086
H	1.45052	-2.22767	-3.95372
H	0.12044	-3.18027	-4.67247
H	0.53755	-3.38133	-2.95188
C	-0.79876	-0.24592	-4.77112
H	-1.51740	0.55351	-4.57933
H	-1.10371	-0.80292	-5.66238
H	0.18552	0.19918	-4.94595
C	-2.33603	-2.08773	-3.06704
C	-3.06462	-2.62477	-4.14202
C	-4.30295	-3.22205	-3.91421
C	-4.81851	-3.29145	-2.61627
C	-4.09663	-2.76392	-1.54513
C	-2.85774	-2.15933	-1.76709
H	-4.48259	-2.82348	-0.53209
H	-2.30149	-1.75409	-0.92949
H	-2.67636	-2.57977	-5.15668
H	-4.86520	-3.63255	-4.74807
H	-5.78311	-3.76030	-2.44281

Y(C_5H_5)$_2$(OPh)

C	-3.18770	0.06701	1.21090
C	-4.58162	0.04407	1.20423
C	-2.47025	0.07917	0.00031
C	-3.18715	0.07002	-1.21062
C	-4.58108	0.04707	-1.20464
C	-5.28968	0.03370	-0.00039
H	-2.63413	0.07640	2.14647
H	-5.11835	0.03436	2.15008
H	-5.11736	0.03975	-2.15078
H	-6.37581	0.01570	-0.00065
H	-2.63318	0.08174	-2.14593
H	0.38481	2.96233	-1.37145
C	1.15853	2.56834	-0.72301
H	2.71008	1.83679	-2.16600
C	2.37656	1.95768	-1.14108
C	1.13781	2.57942	0.69120
O	-1.12967	0.10013	0.00065
H	0.34480	2.98170	1.31047
Y	0.94324	0.00295	0.00028
C	3.11408	1.61085	0.02021
C	2.34251	1.97505	1.15403
H	1.15085	-2.50293	-2.18155
C	1.45008	-2.35631	-1.14924
H	4.09293	1.14799	0.03823
C	0.66939	-2.66628	-0.00609
C	2.71731	-1.88174	-0.70462

H	2.64565	1.86985	2.19010
H	-0.34510	-3.04486	-0.01094
H	3.54870	-1.59608	-1.33811
C	1.44073	-2.36107	1.14450
C	2.71151	-1.88448	0.71209
H	1.13306	-2.51176	2.17372
H	3.53789	-1.60191	1.35350

3.3 Surface and Bulk Oxide Models

3-Coordinated Siloxane Cage

Y	-1.75439	1.90148	0.00220
Si	1.63123	-0.88936	1.48135
Si	1.63316	-0.88493	-1.48312
Si	1.67665	1.70769	0.00158
O	1.86970	-1.55880	-0.00181
O	1.83023	0.73332	1.32830
F	2.69352	-1.46719	2.50908
O	1.83961	0.73664	-1.32624
F	2.86479	2.76912	0.00710
O	0.23547	2.45130	-0.00169
O	0.14072	-1.23402	-2.03737
F	2.69242	-1.46452	-2.51292
O	0.14066	-1.24716	2.03529
Si	-1.41170	-1.07870	1.51716
Si	-1.41250	-1.07389	-1.51954
F	-2.32646	-1.94271	2.49328
O	-1.54171	-1.70159	-0.00217
O	-1.85567	0.49003	1.50396
F	-2.32349	-1.93844	-2.49867
O	-1.86170	0.49336	-1.50211

4-Coordinated Siloxane Cage

Y	-0.05577	-2.02062	-0.00001
O	2.50244	-1.47735	0.00012
Si	3.09254	-1.13791	1.52920
F	2.25491	-2.13566	2.44834
F	4.61052	-1.59033	1.58296
O	2.97171	0.41440	1.90417
Si	2.23007	1.86665	1.60977
F	3.08509	2.97614	2.35016
O	2.28823	2.12208	-0.00013
Si	2.23003	1.86645	-1.61000
F	3.08512	2.97580	-2.35054
O	2.97154	0.41411	-1.90425
O	0.71705	1.85928	-2.21397
Si	-0.50894	0.96616	-1.53704
O	-1.98125	1.22621	-2.21733
Si	-3.42356	0.86728	-1.50018

F	-4.56090	1.44409	-2.44567
O	-3.55909	1.53620	-0.00000
Si	-3.42353	0.86737	1.50021
F	-4.56077	1.44432	2.44573
O	-3.58559	-0.75390	1.32531
Si	-3.46512	-1.74293	0.00011
F	-4.71710	-2.73012	0.00010
O	-1.98115	1.22625	2.21725
Si	-0.50886	0.96623	1.53690
O	-3.58548	-0.75399	-1.32516
O	-0.64068	1.51734	-0.00008
O	0.71710	1.85946	2.21375
Si	3.09246	-1.13813	-1.52903
F	4.61045	-1.59053	-1.58284
F	2.25475	-2.13606	-2.44792
O	-2.06886	-2.55640	0.00018
O	-0.05758	-0.59500	1.51738
O	-0.05775	-0.59510	-1.51748

5-Coordinated Siloxane Cage

Y	-0.05577	-2.02062	-0.00001
O	2.50244	-1.47735	0.00012
Si	3.09254	-1.13791	1.52920
F	2.25491	-2.13566	2.44834
F	4.61052	-1.59033	1.58296
O	2.97171	0.41440	1.90417
Si	2.23007	1.86665	1.60977
F	3.08509	2.97614	2.35016
O	2.28823	2.12208	-0.00013
Si	2.23003	1.86645	-1.61000
F	3.08512	2.97580	-2.35054
O	2.97154	0.41411	-1.90425
O	0.71705	1.85928	-2.21397
Si	-0.50894	0.96616	-1.53704
O	-1.98125	1.22621	-2.21733
Si	-3.42356	0.86728	-1.50018
F	-4.56090	1.44409	-2.44567
O	-3.55909	1.53620	-0.00000
Si	-3.42353	0.86737	1.50021
F	-4.56077	1.44432	2.44573
O	-3.58559	-0.75390	1.32531
Si	-3.46512	-1.74293	0.00011
F	-4.71710	-2.73012	0.00010
O	-1.98115	1.22625	2.21725
Si	-0.50886	0.96623	1.53690
O	-3.58548	-0.75399	-1.32516
O	-0.64068	1.51734	-0.00008
O	0.71710	1.85946	2.21375
Si	3.09246	-1.13813	-1.52903
F	4.61045	-1.59053	-1.58284

F	2.25475	-2.13606	-2.44792
O	-2.06886	-2.55640	0.00018
O	-0.05758	-0.59500	1.51738
O	-0.05775	-0.59510	-1.51748

***trans*-Y(OSiF$_3$)$_3$(O(SiF$_3$)$_2$)$_2$**

Y	0.00668	-0.00872	0.35769
O	-2.26984	0.30150	-0.70243
O	2.46866	-0.34090	0.75584
Si	3.45729	0.97324	0.41592
Si	2.88393	-1.93373	1.00809
Si	-3.25119	1.39525	0.07772
Si	-2.66015	-0.82122	-1.88502
O	0.14328	-0.76343	-1.61490
O	0.79940	1.93069	0.57642
O	-0.79803	-1.06735	1.98297
F	-2.25268	-2.26525	-1.39543
F	-2.07326	-0.44779	-3.30136
F	-4.24190	-0.73049	-1.98912
F	-2.32203	1.83209	1.29627
F	-4.58997	0.76007	0.60474
F	-3.58182	2.61141	-0.86620
F	1.54729	-2.69917	0.61325
F	3.12731	1.53434	-1.02148
F	4.92108	0.35904	0.40429
F	3.41207	2.06210	1.55590
Si	0.51123	3.49671	0.38936
F	1.71352	4.24398	-0.33840
F	0.24019	4.25353	1.76268
F	-0.79842	3.69094	-0.51751
Si	1.18776	-1.18861	-2.75136
F	0.76179	-2.51683	-3.51523
F	2.61944	-1.47475	-2.06919
F	1.42771	-0.05794	-3.84387
Si	-2.06143	-1.91117	2.48309
F	-2.51677	-1.54643	3.96352
F	-1.82712	-3.48483	2.42985
F	-3.31634	-1.59520	1.52439
F	3.20393	-2.16071	2.53632
F	4.10685	-2.40041	0.13742

***mer*-Y(OSiF$_3$)$_3$(O(SiF$_3$)$_2$)$_3$**

Y	-0.01109	-0.43020	0.31201
O	0.37053	1.37681	1.38870
O	0.96778	1.83356	-1.31142
O	0.34849	-1.35174	-1.59825
O	-0.98869	-1.86843	1.43693
Si	0.24696	2.30795	-2.71053
F	0.80855	3.72478	-3.13539

F	-1.31040	2.44211	-2.41948
F	0.48213	1.25967	-3.86361
Si	2.20870	2.52846	-0.46942
F	1.73476	3.73103	0.43837
F	3.24240	3.10258	-1.52637
F	2.97001	1.39908	0.35174
Si	0.56870	1.99085	2.86125
F	0.24476	0.92365	4.00186
F	-0.37211	3.25220	3.11771
F	2.07830	2.45889	3.08700
Si	-2.36511	-2.42330	2.04408
F	-2.37177	-2.45792	3.63417
F	-2.71959	-3.88739	1.53481
F	-3.58010	-1.46735	1.59569
Si	-0.43691	-2.56364	-2.30272
F	-0.51257	-2.44016	-3.88653
F	-1.94952	-2.59290	-1.74514
F	0.17540	-3.99342	-1.96333
O	2.34960	-1.39008	0.29712
O	-2.31065	0.57998	-0.20398
Si	3.04752	-1.57156	1.79708
F	3.40223	-3.08706	2.05061
F	1.89120	-1.09020	2.77257
F	4.32935	-0.67448	1.97111
Si	3.08947	-1.57131	-1.19498
F	2.93691	-0.25713	-2.06284
F	2.68222	-2.88059	-1.97235
F	4.62615	-1.72525	-0.80993
Si	-3.24433	0.24220	-1.55892
F	-4.23120	-0.95174	-1.29107
F	-2.24462	-0.08920	-2.73922
F	-4.07020	1.54808	-1.89506
Si	-2.88601	1.56485	1.02948
F	-2.35148	1.00338	2.40681
F	-4.46460	1.51591	0.98035
F	-2.38950	3.04170	0.79244

***fac*-$Y(OSiF_3)_3(O(SiF_3)_2)_3$**

Y	0.00780	0.00271	0.32453
O	1.70372	-0.48456	1.56609
O	-1.19094	-1.22025	1.44608
O	-1.80738	0.54279	-0.85458
O	1.40891	1.28488	-0.81568
O	-0.43161	1.68023	1.61644
O	0.41065	-1.86695	-0.81706
Si	-3.25958	-0.06370	-0.16160
F	-4.36337	0.68073	-1.03225
F	-3.50297	0.29144	1.34595
F	-3.32537	-1.60787	-0.49387
Si	-1.97269	1.53795	-2.21001

F	-0.49195	1.67927	-2.77090
F	-2.52742	2.95593	-1.82562
F	-2.86783	0.84753	-3.30680
Si	2.35222	0.92432	-2.17195
F	2.21364	2.04672	-3.26851
F	1.72451	-0.42266	-2.73658
F	3.85511	0.68457	-1.78446
Si	1.62461	2.84847	-0.12827
F	0.31260	3.66563	-0.45907
F	2.81629	3.42794	-1.00745
F	2.06017	2.88685	1.37612
Si	3.14682	-0.11645	2.13069
F	3.90995	0.87090	1.10658
F	4.08923	-1.39877	2.27749
F	3.13349	0.61559	3.54329
Si	-1.67426	-2.54331	2.20524
F	-1.28519	-3.84118	1.34187
F	-3.26162	-2.58103	2.37424
F	-1.03595	-2.72587	3.64905
Si	-0.36898	-2.53053	-2.15964
F	0.66988	-2.98658	-3.25264
F	-1.23394	-1.33845	-2.75644
F	-1.31518	-3.70952	-1.73020
Si	1.65071	-2.82347	-0.10367
F	1.55627	-4.15372	-0.97374
Si	-1.48969	2.75557	2.12507
F	-2.69672	2.89964	1.06083
F	-0.86138	4.21877	2.26114
F	-2.16162	2.40648	3.52513
F	1.42896	-3.22651	1.39544
F	3.02936	-2.12346	-0.43071

4 NMR Shielding Tensors and NCS Analysis - Graphical Comparison

4.1 $Y(CH_3)_3$, $Y(CH_3)_2(NH_2)$, $Y(CH_3)(NH_2)_2$ and $Y(NH_2)_3$

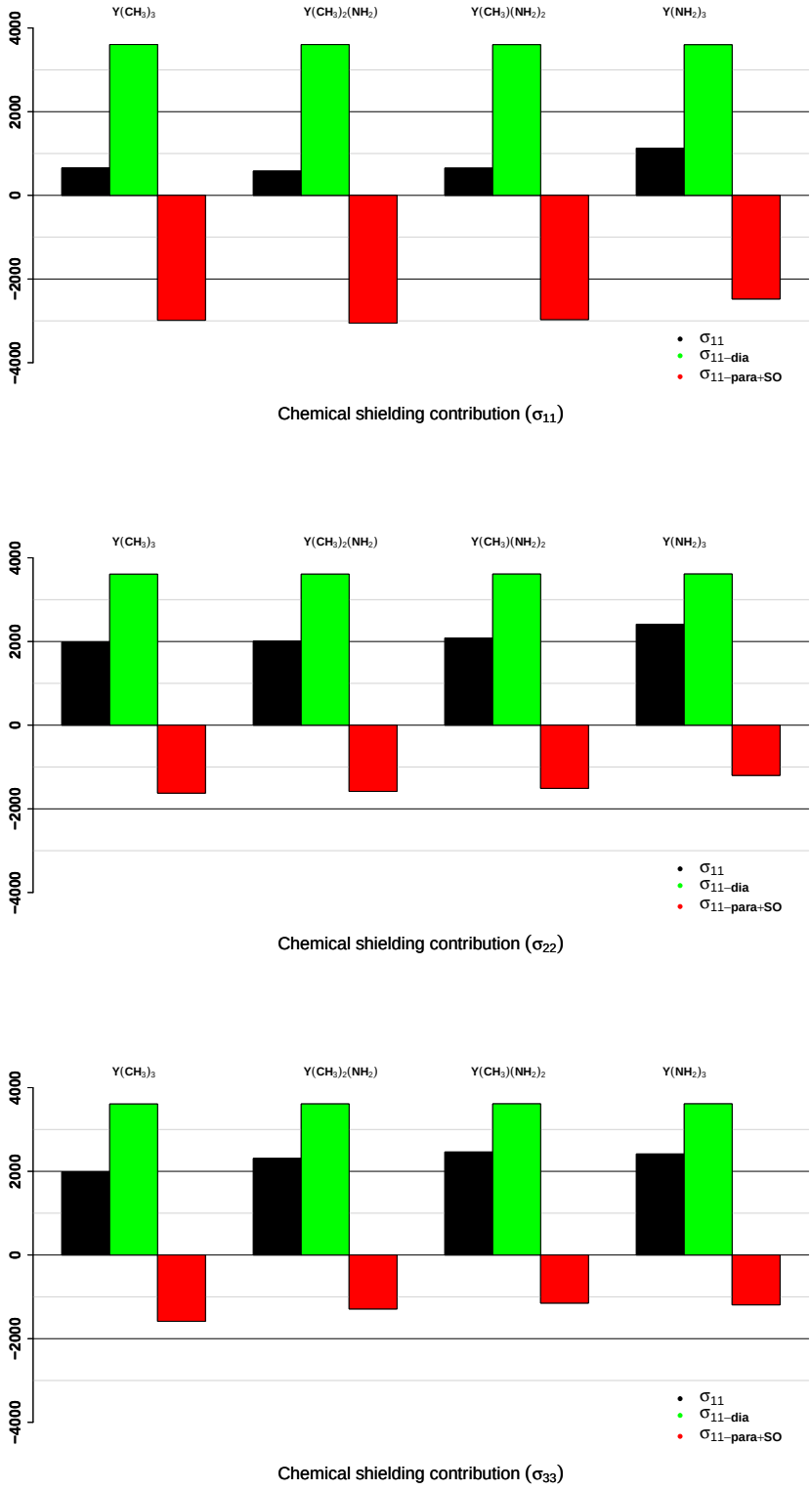
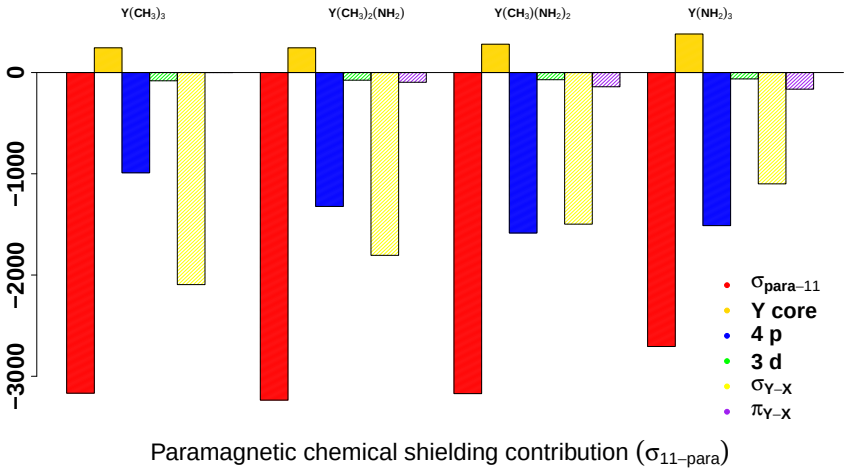
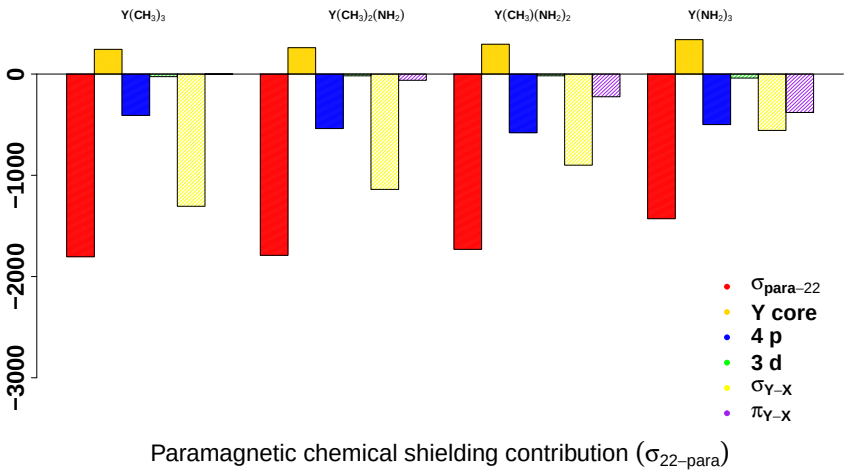


Figure S3: Diamagnetic, paramagnetic and spin-orbit contribution to the chemical shielding tensor.





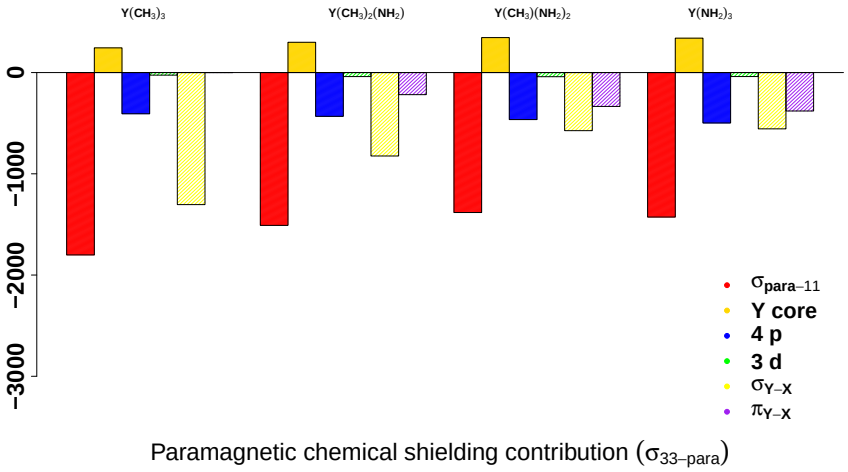
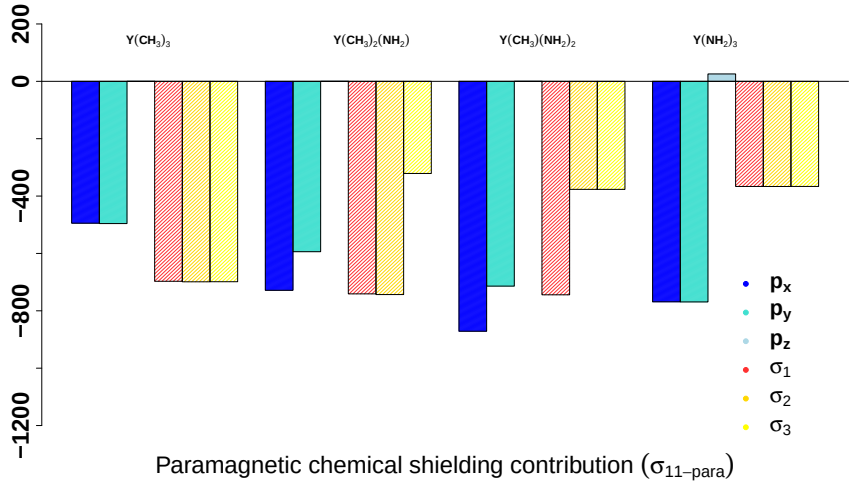
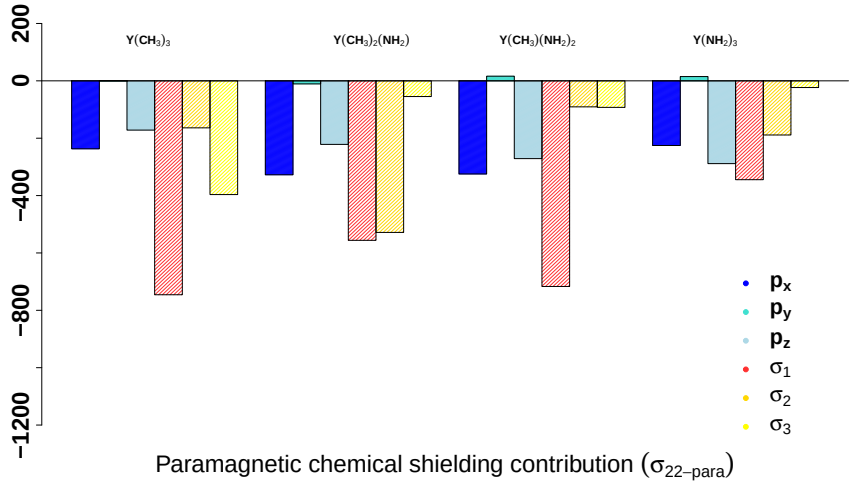


Figure S4: Orbital contributions to the paramagnetic shielding tensor.





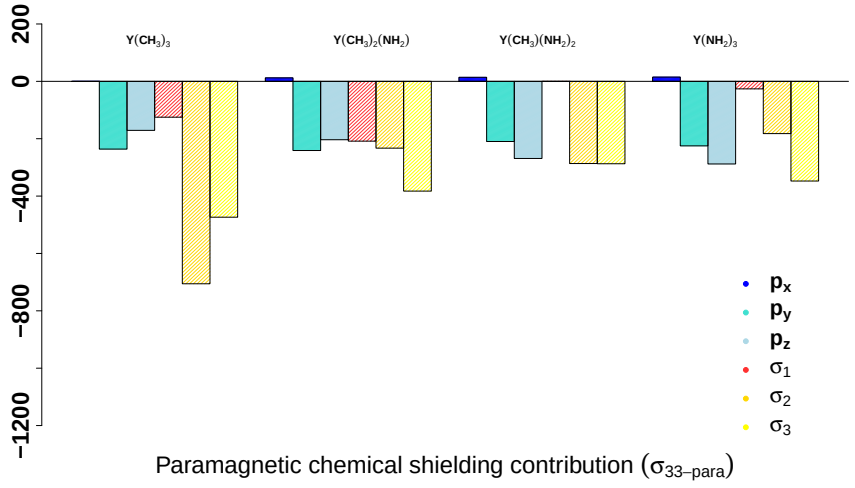


Figure S5: $4p_x$, $4p_y$, $4p_z$, σ_{Y-X_1}, σ_{Y-X_2} and σ_{Y-X_3} contributions to the paramagnetic shielding tensor.

4.2 Orbital Rotation Model: Alkyl-Amido-Series

The situation for $Y(CH_3)_2(NH_2)$ and $Y(CH_3)(NH_2)_2$ is illustrated below. As σ_{22} is placed along the yttrium-amido bond for $Y(CH_3)_2(NH_2)$ - resulting in a 60° angle for both methyl ligands with respect to L_x - one obtains two moderate contributions from σ_{Y-Me1} and σ_{Y-Me2}. Those contributions decrease substantially as the angle is reduced to 30° when L_y is applied. Although the amido-ligand is found to have a perfect 90° relationship now, the contribution is lower compared to $Y(CH_3)_3$ due to the low lying σ-orbital in $Y(CH_3)_2(NH_2)$.
For $Y(CH_3)(NH_2)_2$, σ_{22} is placed perpendicular to the yttrium-methyl bond. This can be understood as σ_{22} has to give the second largest contribution ($\sigma_{33} < \sigma_{22} < \sigma_{11}$) which is achieved by placing the ligand with the highest lying σ-orbital perpendicular to the y-axis. For σ_{33} no contribution from the methyl ligand and two small contributions from the amido ligands are observed, because of their low lying $\sigma-$orbitals and the non-perfect 60° arrangement.

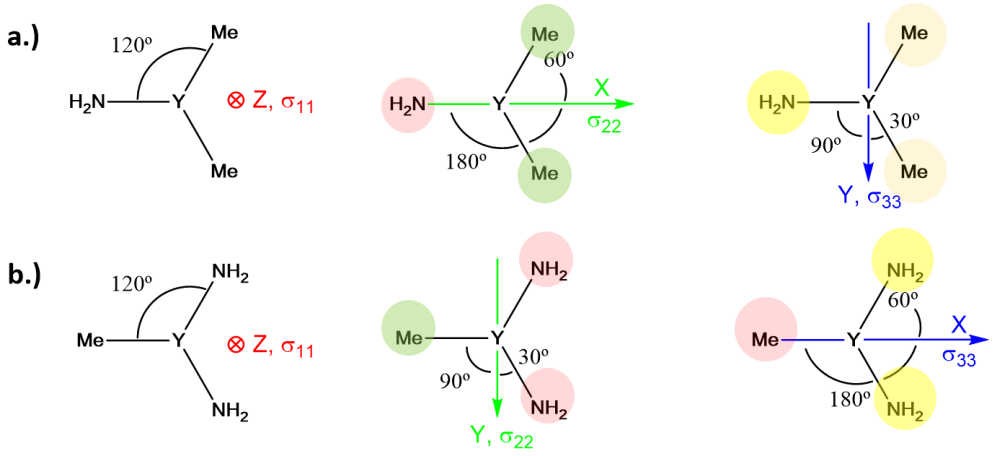


Figure S6: *Top:* $Y(CH_3)_2(NH_2)$, *Bottom:* $Y(CH_3(NH_2)_2$. Direction of L_z (left), L_y (middle) and L_x (right) with respect to the three σ_{Y-X}-orbitals.

4.3 $Y(CH_3)_3$, $Y(NH_2)_3$, YCl_3 and $Y(OH)_3$

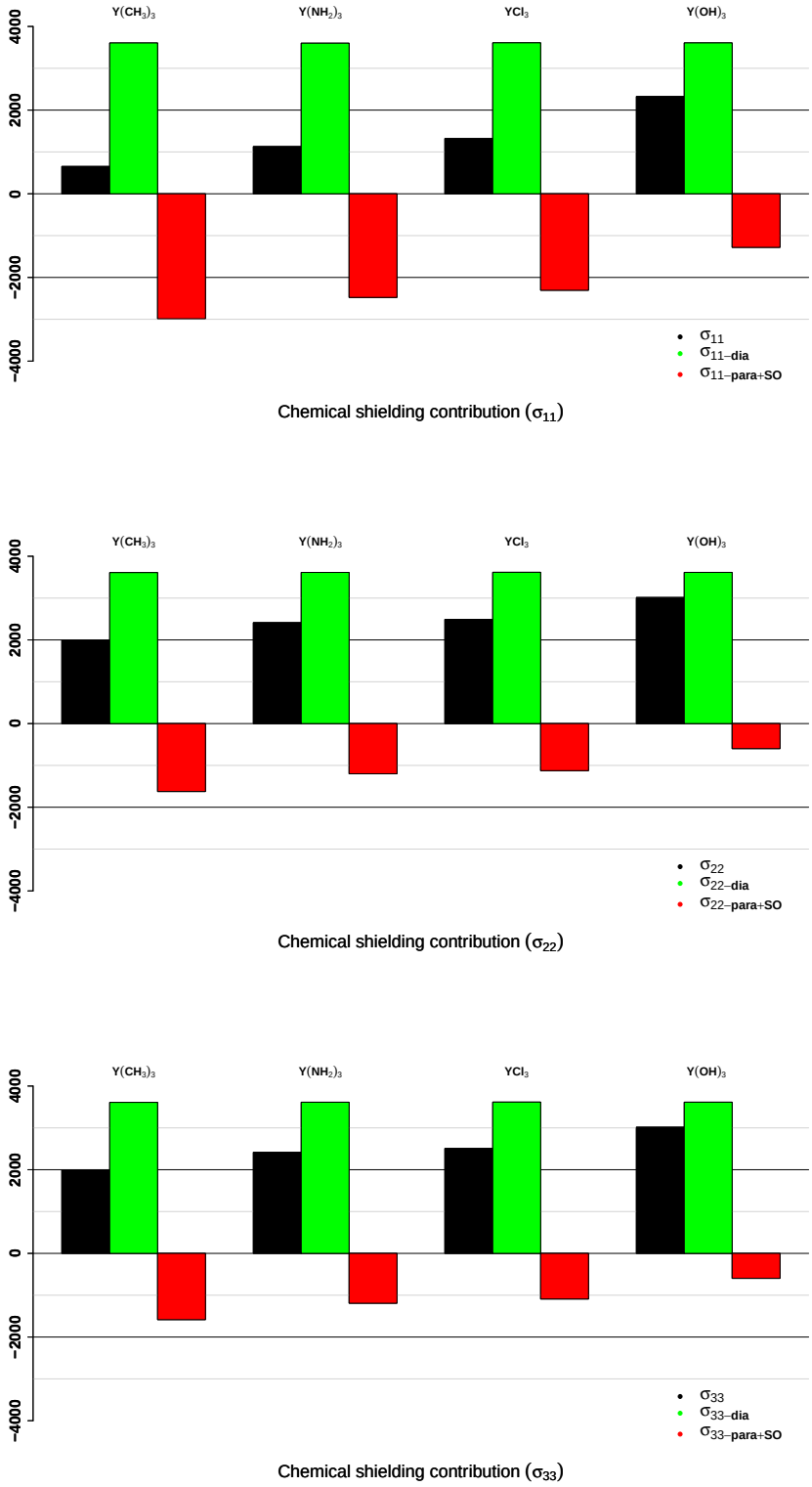
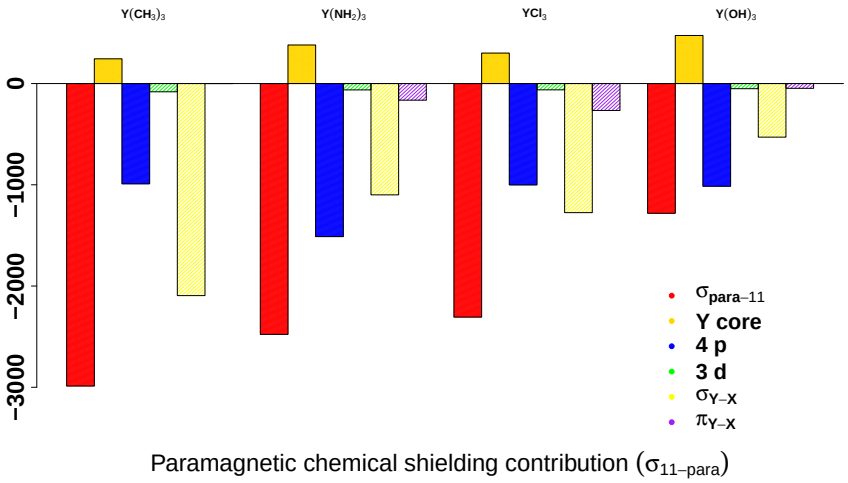
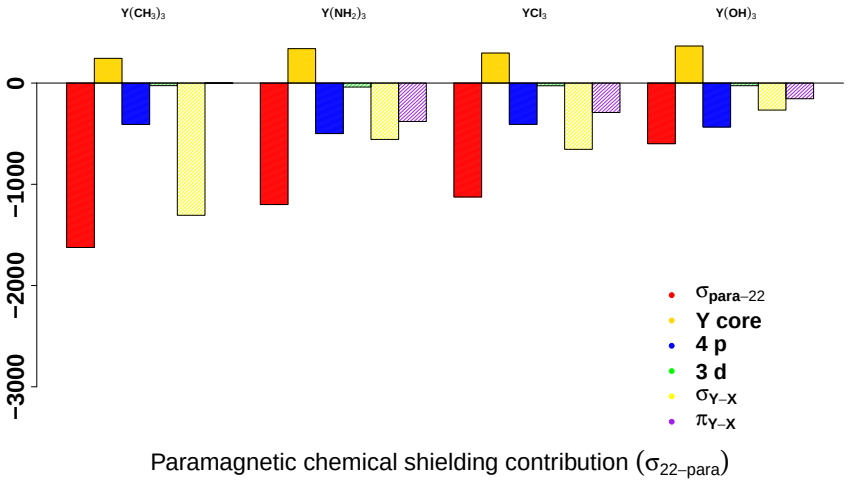


Figure S7: Diamagnetic, paramagnetic and spin-orbit contribution to the chemical shielding tensor.





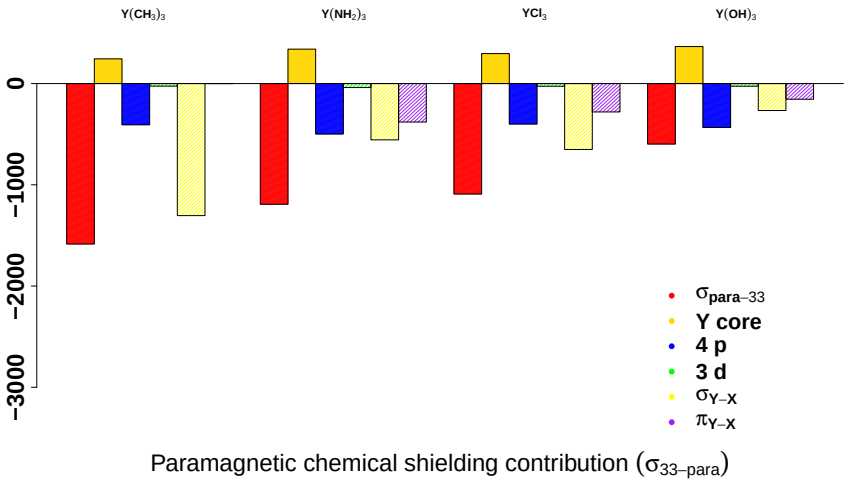
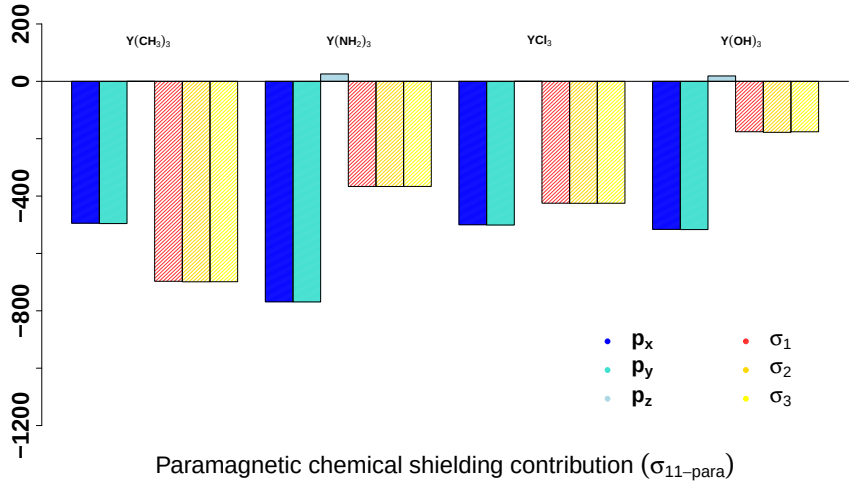
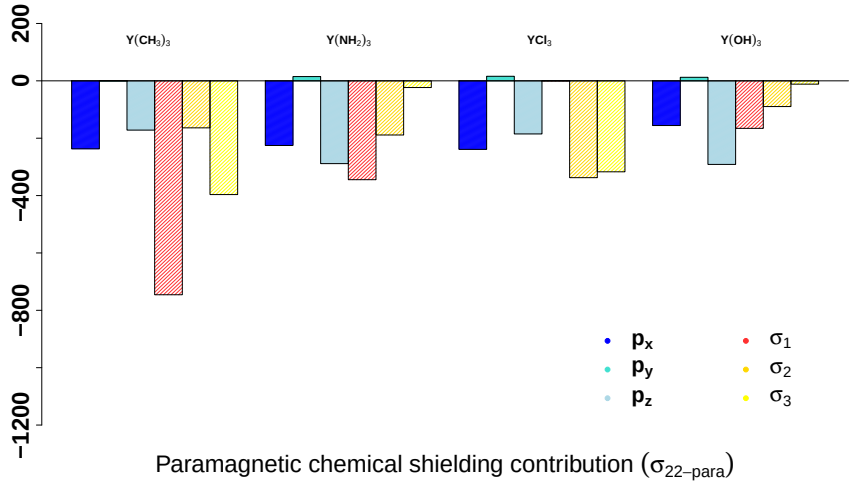


Figure S8: Orbital contributions to the paramagnetic shielding tensor.





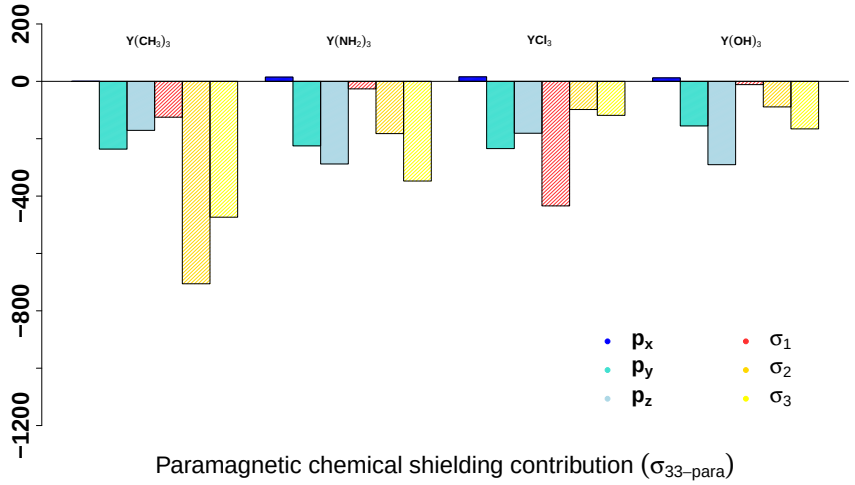


Figure S9: $4p_x$, $4p_y$, $4p_z$, σ_{Y-X_1}, σ_{Y-X_2} and σ_{Y-X_3} contributions to the paramagnetic shielding tensor.

4.4 $Y(NH_2)_3$, $Y(N(CH_3)_2)_3$, $Y(OH)_3$ and $Y(OCH3)_3$

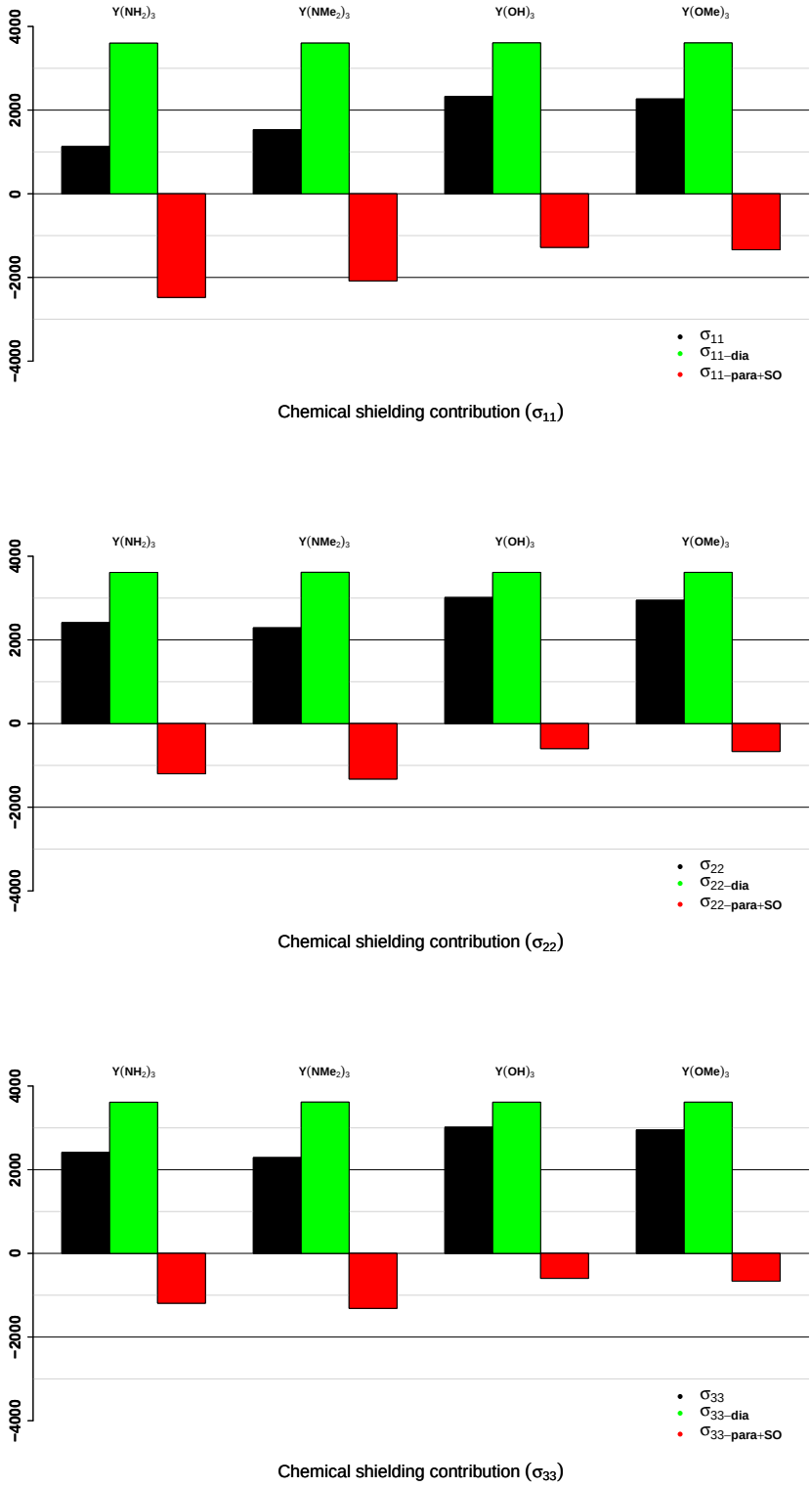
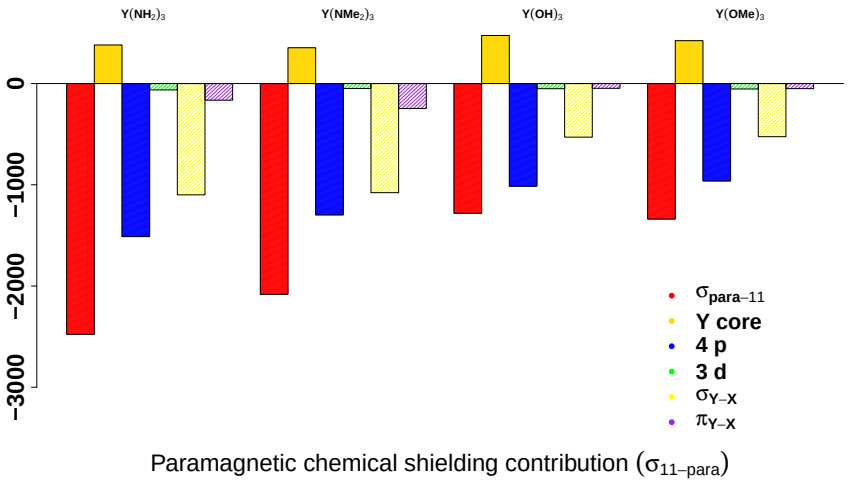
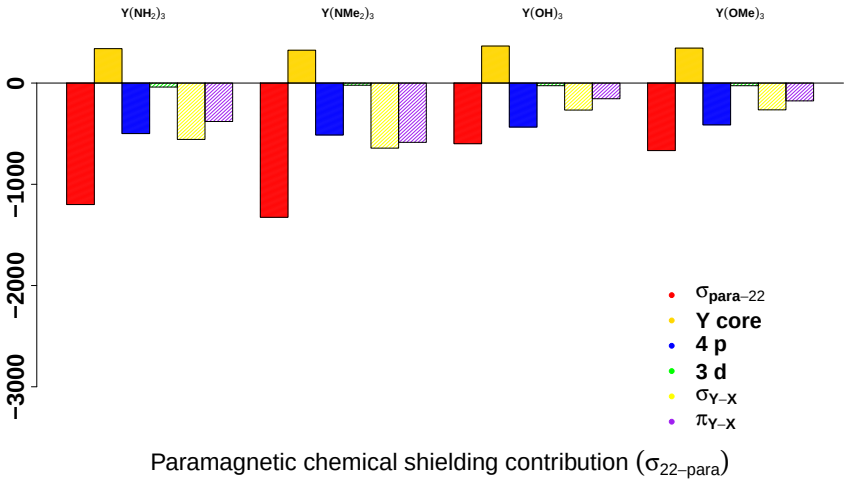


Figure S10: Diamagnetic, paramagnetic and spin-orbit contribution to the chemical shielding tensor.





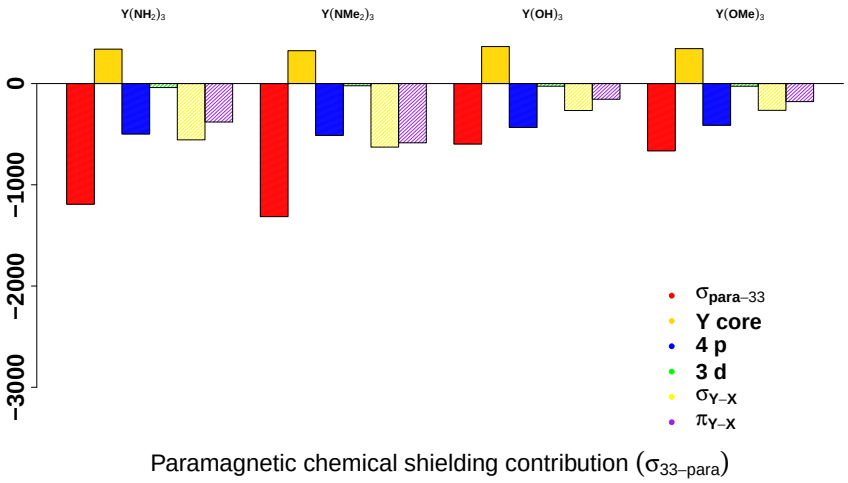


Figure S11: Orbital contributions to the paramagnetic shielding tensor.

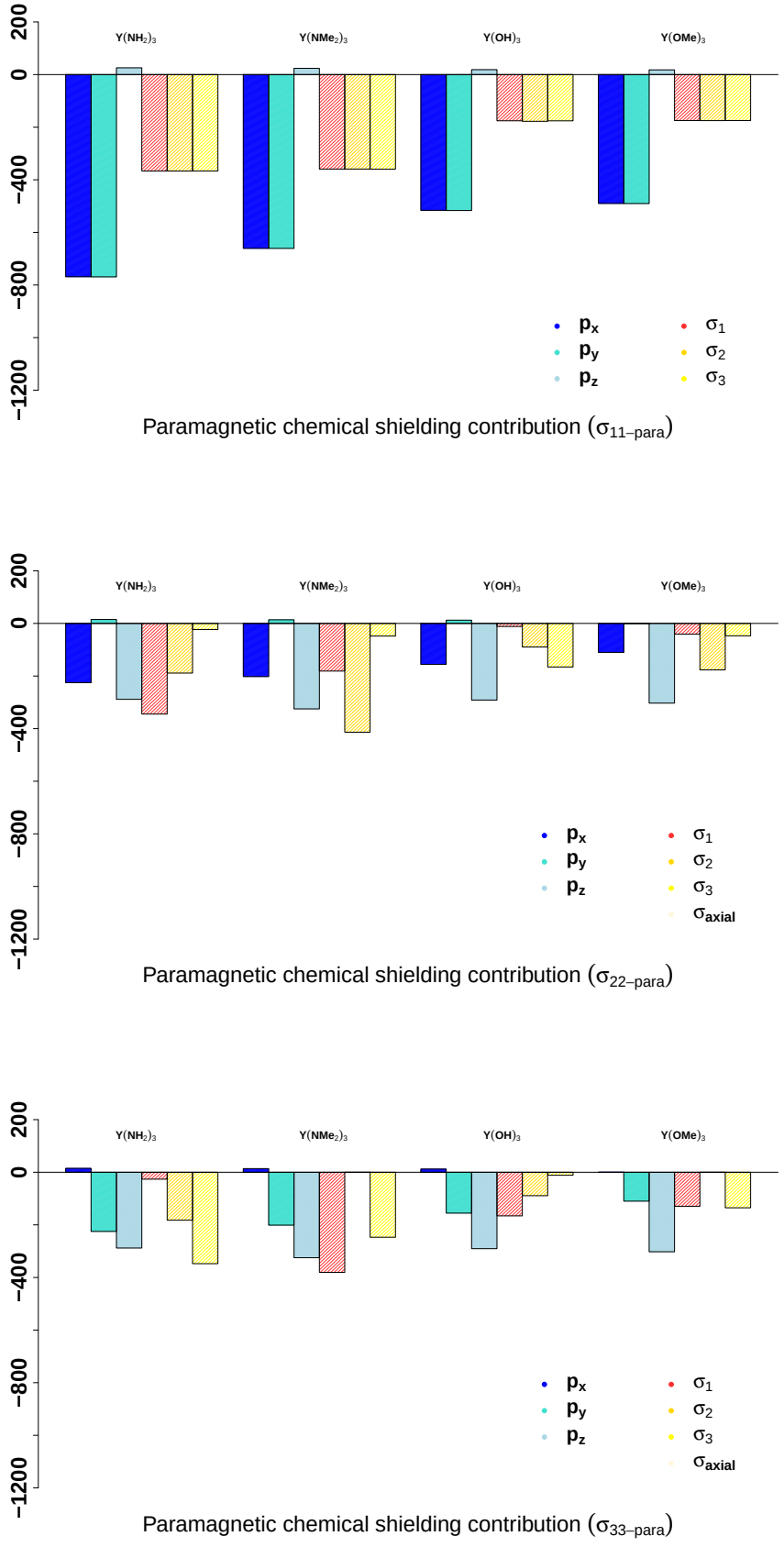


Figure S12: $4p_x$, $4p_y$, $4p_z$, σ_{Y-X_1}, σ_{Y-X_2} and σ_{Y-X_3} contributions to the paramagnetic shielding tensor.

4.5 $Y(CH_3)_3$, $Y(CH_3)_3(thf)$, *cis*-$Y(CH_3)_3(thf)_2$ and *trans*-$Y(CH_3)_3(thf)_2$

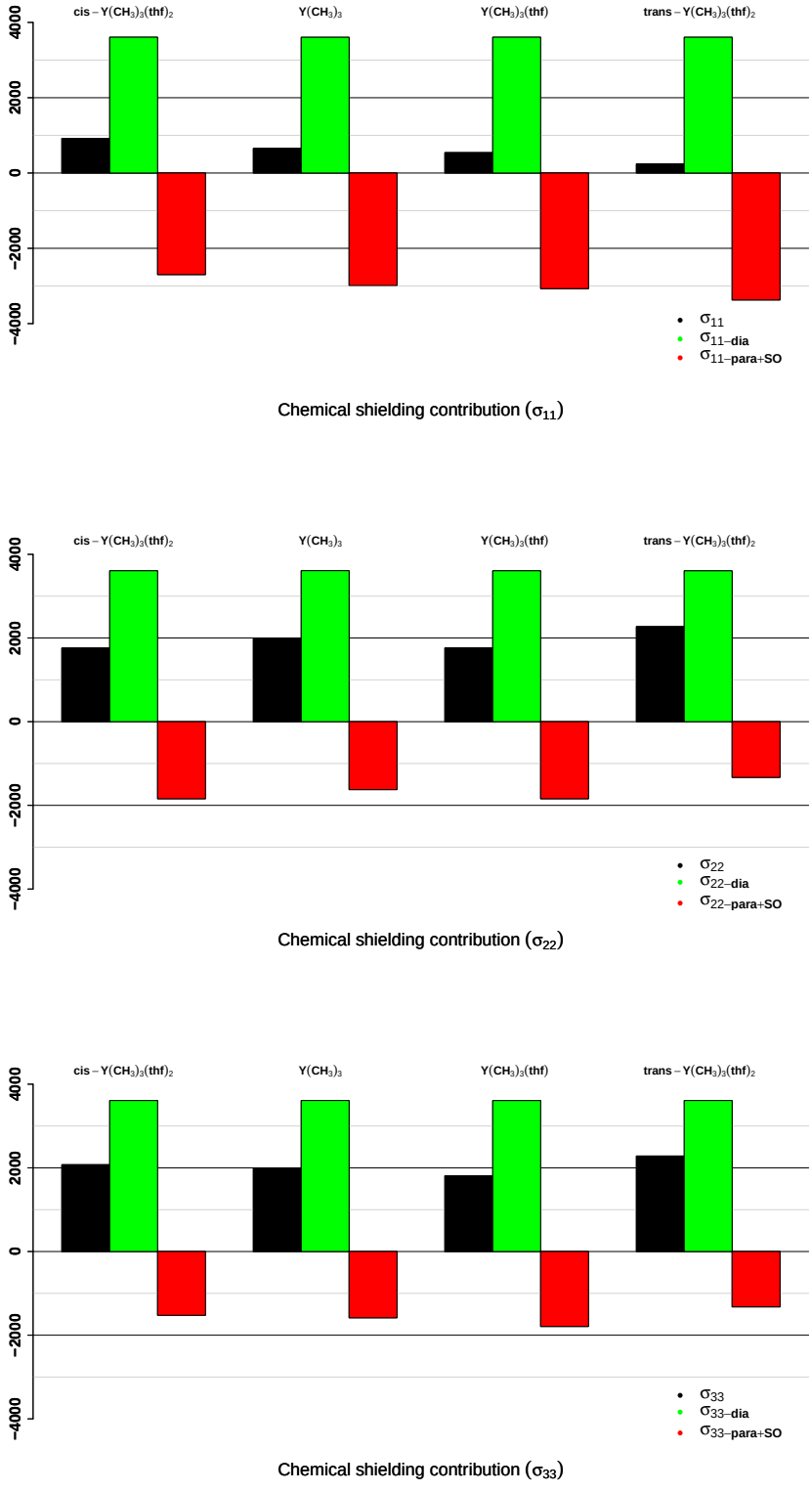
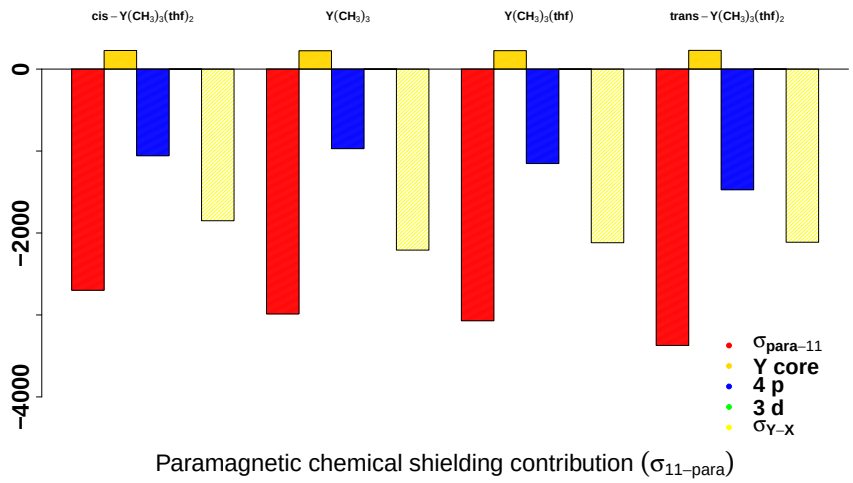
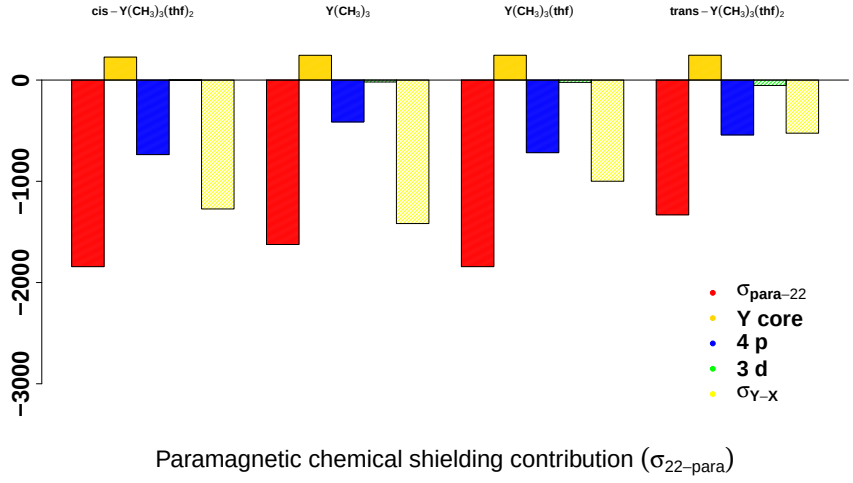


Figure S13: Diamagnetic, paramagnetic and spin-orbit contribution to the chemical shielding tensor.





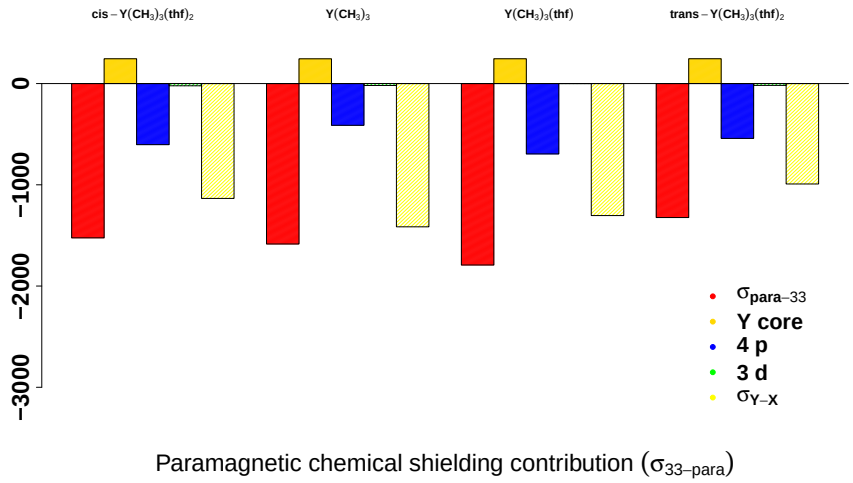


Figure S14: Orbital contributions to the paramagnetic shielding tensor.

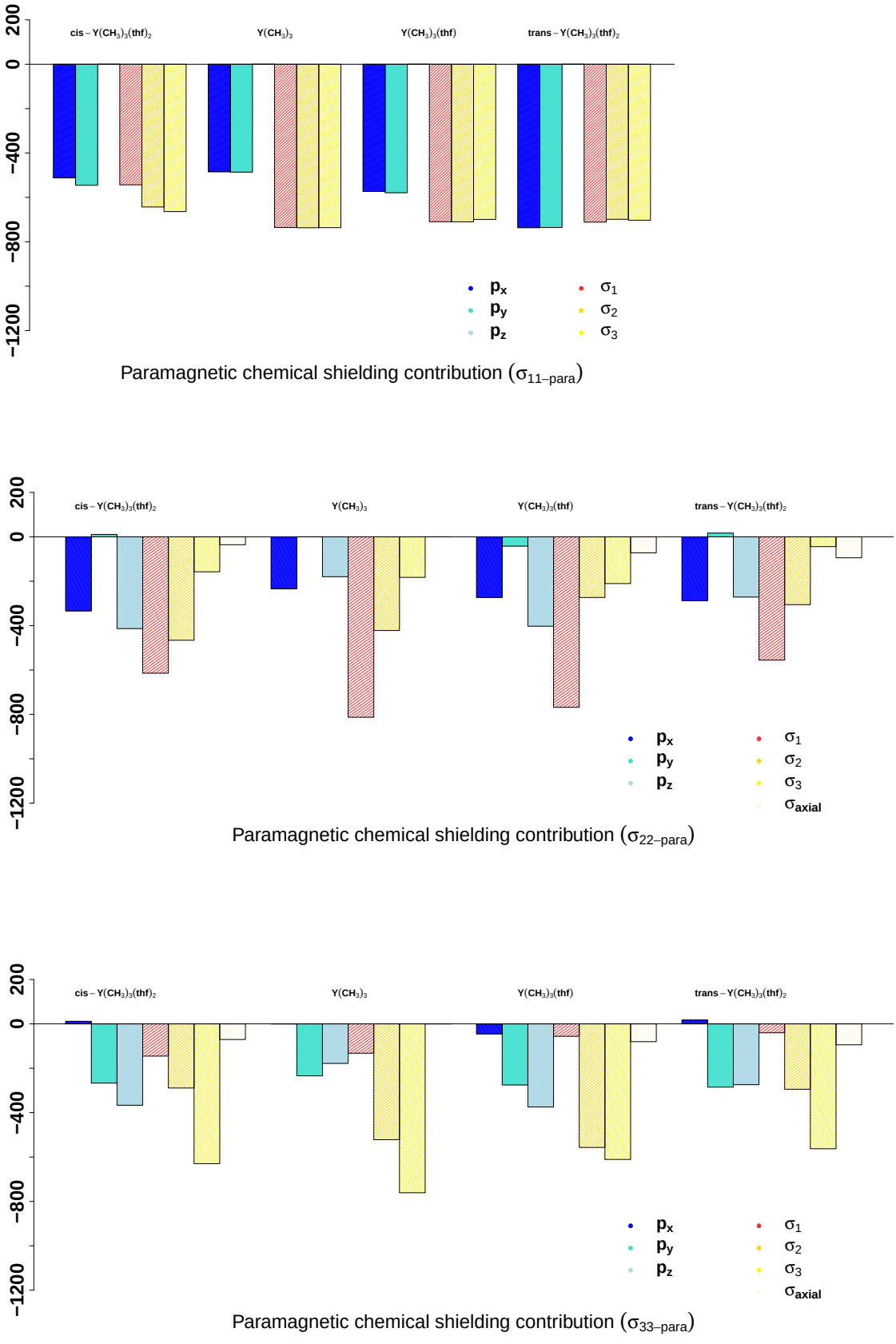


Figure S15: $4p_x$, $4p_y$, $4p_z$, σ_{Y-X_1}, σ_{Y-X_2} and σ_{Y-X_3} contributions to the paramagnetic shielding tensor.

4.6 Reported Organoyttrium Compounds

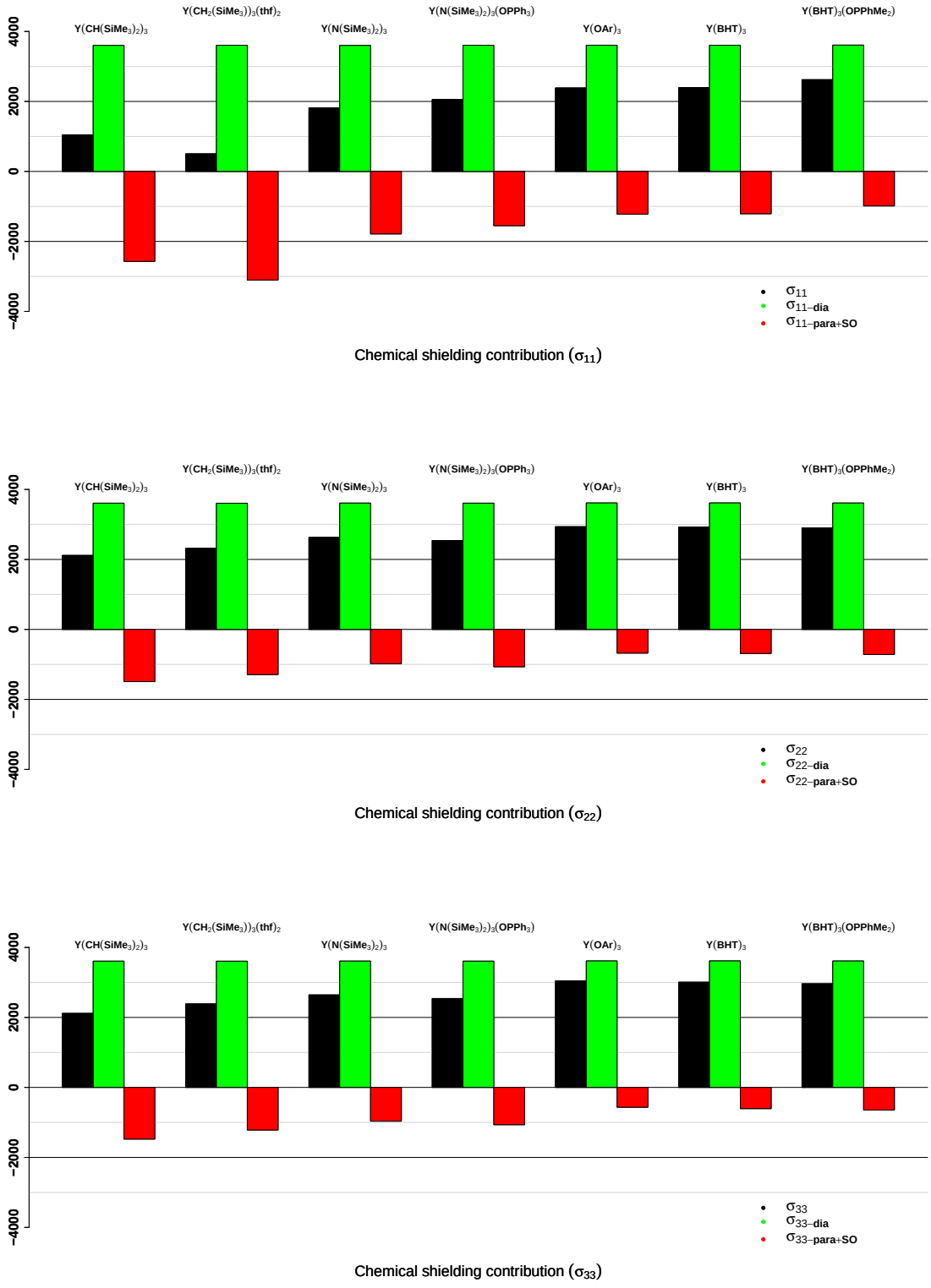
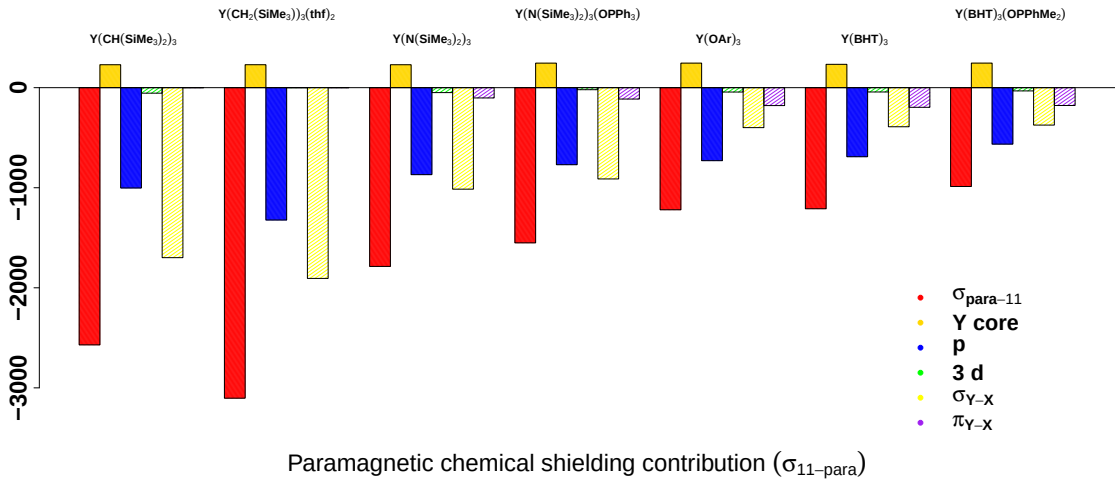
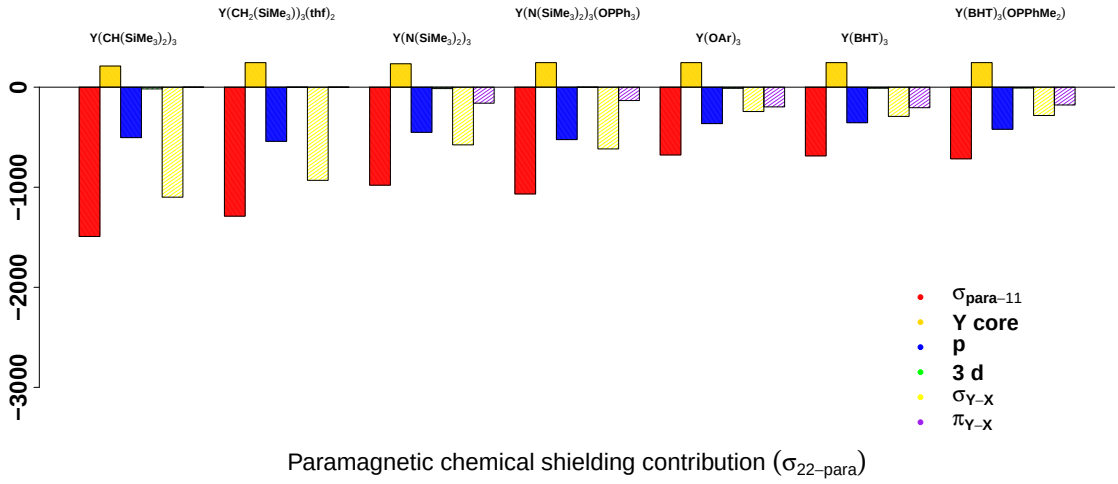


Figure S16: Diamagnetic, paramagnetic and spin-orbit contribution to the chemical shielding tensor.





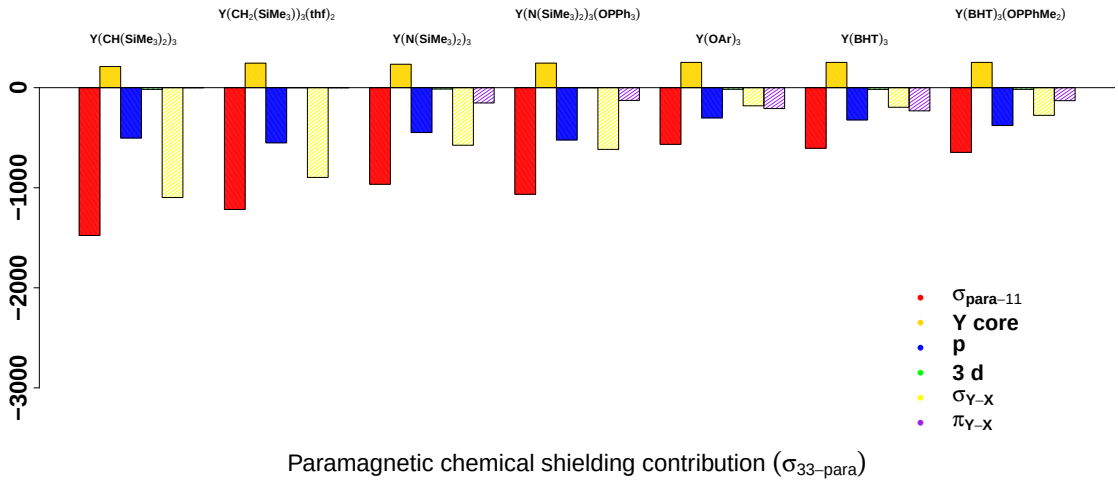
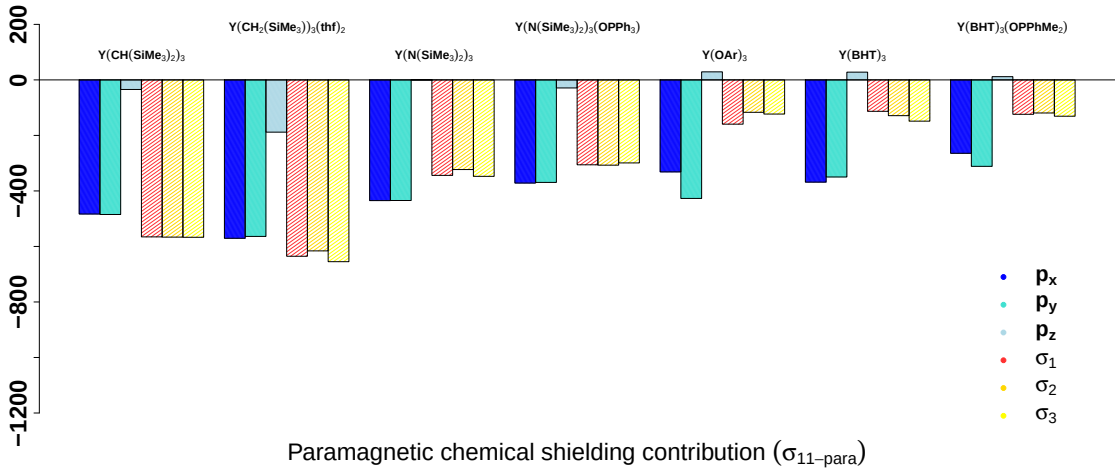
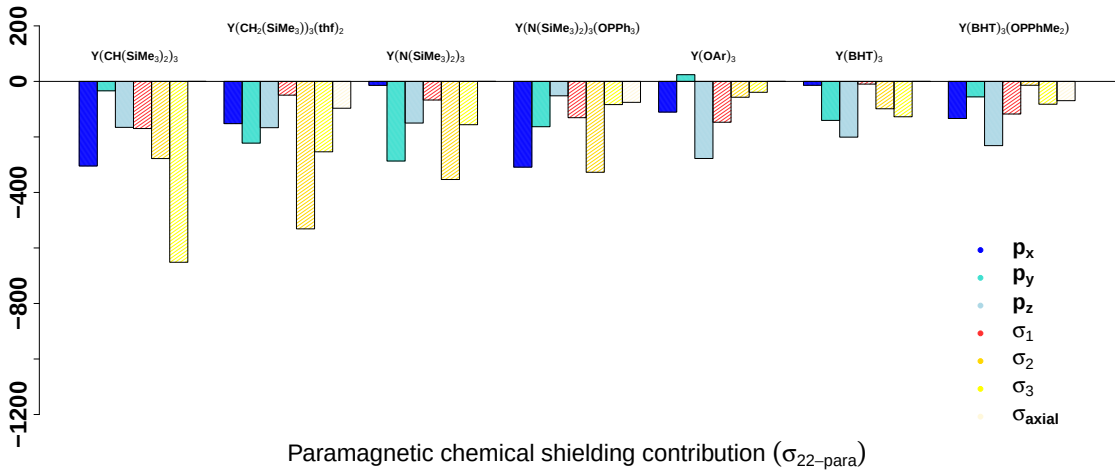


Figure S17: Orbital contributions to the paramagnetic shielding tensor.





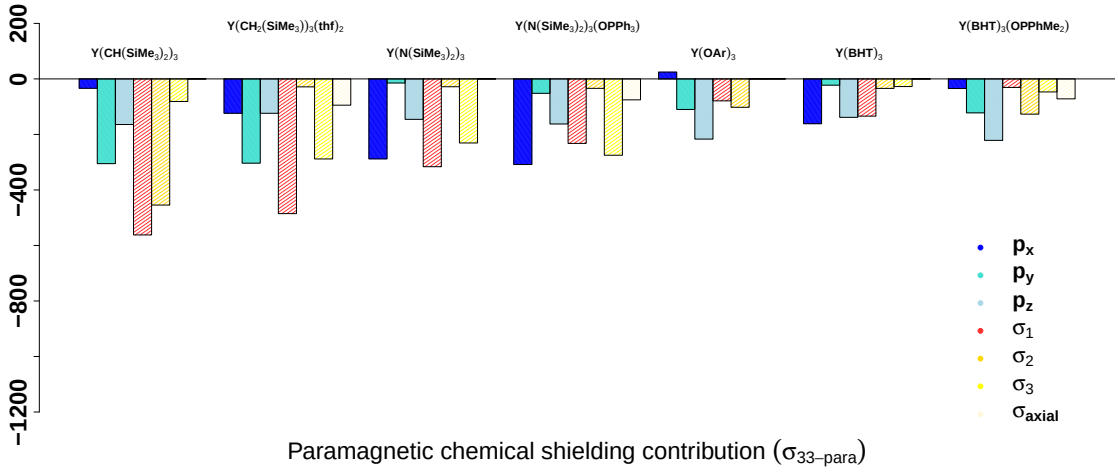


Figure S18: $4p_x$, $4p_y$, $4p_z$, σ_{Y-X_1}, σ_{Y-X_2} and σ_{Y-X_3} contributions to the paramagnetic shielding tensor.

5 NCS Analysis: Orbital Contributions - Values

5.1 Organoyttrium Model Compounds

$Y(CH_3)_3$

Table S1: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
211.952	CR (1)	Y	1	1 s
32.318	CR (2)	Y	1	2 s
-494.610	CR (7)	Y	1	4 p_x
-495.857	CR (10)	Y	1	4 p_y
-40.736	CR (14)	Y	1	3 d_{xy}
-40.650	CR (17)	Y	1	3 $d_{x^2-y^2}$
-697.095	BD (1)	Y	1- C 2	σ_{Y-C}
-698.890	BD (1)	Y	1- C 3	σ_{Y-C}
-698.601	BD (1)	Y	1- C 4	σ_{Y-C}

Table S2: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
211.904	CR (1)	Y	1	1 s
32.110	CR (2)	Y	1	2 s
-30.421	CR (4)	Y	1	4 s
-236.977	CR (7)	Y	1	4 p_x
-171.724	CR (13)	Y	1	4 p_z
-25.537	CR (15)	Y	1	3 d_{xz}
-745.772	BD (1)	Y	1- C 2	σ_{Y-C}
-163.904	BD (1)	Y	1- C 3	σ_{Y-C}
-396.478	BD (1)	Y	1- C 4	σ_{Y-C}
-7.987	BD (1)	C	2- H 5	σ_{C-H}
-16.217	BD (1)	C	2- H 7	σ_{C-H}
28.319	RY (13)	Y	1	5 sp
230.159	RY (18)	Y	1	5 p_z
-27.839	RY (22)	Y	1	5 p_x
-19.514	RY (23)	Y	1	5 s
-199.948	RY (26)	Y	1	5 s

Table S3: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
211.905	CR (1)	Y	1	1 s
32.114	CR (2)	Y	1	2 s
-30.302	CR (4)	Y	1	4 s
-236.161	CR (10)	Y	1	4 p_y
-170.886	CR (13)	Y	1	4 p_z
-25.418	CR (16)	Y	1	3 d_{yz}
-125.002	BD (1)	Y	1- C 2	σ_{Y-C}
-705.720	BD (1)	Y	1- C 3	σ_{Y-C}
-473.619	BD (1)	Y	1- C 4	σ_{Y-C}
-13.799	BD (1)	C	3- H 9	σ_{C-H}
-12.696	BD (1)	C	4- H 12	σ_{C-H}
-6.027	BD (1)	C	4- H 13	σ_{C-H}
27.958	RY (13)	Y	1	5 sp
230.552	RY (18)	Y	1	5 p_z
-17.073	RY (20)	Y	1	5 sp^3
-28.215	RY (22)	Y	1	5 p_x
-17.678	RY (23)	Y	1	5 s
-202.860	RY (26)	Y	1	5 s

$Y(CH_3)_2(NH_2)$

Table S4: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
208.565	CR (1)	Y	1	1 s
35.609	CR (2)	Y	1	2 s
-728.578	CR (7)	Y	1	4 p_x
-593.941	CR (10)	Y	1	4 p_y
-40.317	CR (14)	Y	1	3 d_{xy}
-35.178	CR (17)	Y	1	3 $d_{x^2-y^2}$
-740.964	BD (1)	Y	1- C 2	σ_{Y-C}
-743.359	BD (1)	Y	1- C 3	σ_{Y-C}
-321.207	BD (1)	Y	1- N 12	σ_{Y-N}
-96.064	BD (2)	Y	1- N 12	π_{Y-N}

Table S5: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
208.443	CR (1)	Y	1	1 s
35.669	CR (2)	Y	1	2 s
-28.132	CR (4)	Y	1	4 s
-327.556	CR (7)	Y	1	4 p_x
16.430	CR (9)	Y	1	3 p_y
10.656	CR (10)	Y	1	4 p_y
-221.565	CR (13)	Y	1	4 p_z
-17.476	CR (15)	Y	1	3 d_{xz}
-556.039	BD (1)	Y	1- C 2	σ_{Y-C}
-528.456	BD (1)	Y	1- C 3	σ_{Y-C}
-54.730	BD (1)	Y	1- N 12	σ_{Y-N}
-61.587	BD (2)	Y	1- N 12	π_{Y-N}
-9.348	BD (1)	C	4- H 5	σ_{C-H}
-12.609	BD (1)	C	4- H 6	σ_{C-H}
-7.430	BD (1)	C	4- H 9	σ_{C-H}
16.218	RY (11)	Y	1	5 spd

Table S6: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
208.545	CR (1)	Y	1	1 s
35.859	CR (2)	Y	1	2 s
-19.656	CR (4)	Y	1	4 s
17.237	CR (5)	Y	1	2 p_x
16.158	CR (6)	Y	1	3 p_x
12.214	CR (7)	Y	1	4 p_x
-241.155	CR (10)	Y	1	4 p_y
21.208	CR (12)	Y	1	3 p_z
-203.520	CR (13)	Y	1	4 p_z
-24.408	CR (16)	Y	1	3 d_{yz}
-15.269	CR (18)	Y	1	3 d_{z^2}
-208.493	BD (1)	Y	1- C 2	σ_{Y-C}
-232.897	BD (1)	Y	1- C 3	σ_{Y-C}
-382.652	BD (1)	Y	1- N 12	σ_{Y-N}
-218.207	BD (2)	Y	1- N 12	π_{Y-N}
-14.912	BD (1)	H	10- N 12	σ_{C-H}
-14.951	BD (1)	H	11- N 12	σ_{C-H}

$Y(CH_3)(NH_2)_2$

Table S7: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
203.512	CR (1)	Y	1	1 s
40.690	CR (2)	Y	1	2 s
-871.236	CR (7)	Y	1	4 p_x
-713.920	CR (10)	Y	1	4 p_y
35.686	CR (11)	Y	1	2 p_z
-33.616	CR (14)	Y	1	3 d_{xy}
-37.185	CR (17)	Y	1	3 $d_{x^2-y^2}$
-744.240	BD (1)	Y	1- C 2	σ_{Y-C}
-376.616	BD (1)	Y	1- N 10	σ_{Y-N}
-69.985	BD (2)	Y	1- N 10	π_{Y-N}
-376.661	BD (1)	Y	1- N 11	σ_{Y-N}
-70.409	BD (2)	Y	1- N 11	π_{Y-N}

Table S8: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
203.345	CR (1)	Y	1	1 s
40.931	CR (2)	Y	1	2 s
-23.421	CR (4)	Y	1	4 s
-324.708	CR (7)	Y	1	4 p_x
16.844	CR (8)	Y	1	2 p_y
17.524	CR (9)	Y	1	3 p_y
16.192	CR (10)	Y	1	4 p_y
15.903	CR (12)	Y	1	3 p_z
-271.137	CR (13)	Y	1	4 p_z
-17.107	CR (15)	Y	1	3 d_{xz}
-716.885	BD (1)	Y	1- C 2	σ_{Y-C}
-90.701	BD (1)	Y	1- N 10	σ_{Y-N}
-112.352	BD (2)	Y	1- N 10	π_{Y-N}
-92.508	BD (1)	Y	1- N 11	σ_{Y-N}
-111.795	BD (2)	Y	1- N 11	π_{Y-N}
-12.008	BD (1)	C	2- H 4	σ_{C-H}
-19.008	RY (14)	Y	1	5 sd
29.294	RY (20)	Y	1	5 s
-48.325	RY (35)	Y	1	5 d

Table S9: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
203.413	CR (1)	Y	1	1 s
41.303	CR (2)	Y	1	2 s
22.686	CR (5)	Y	1	2 p_x
17.628	CR (6)	Y	1	3 p_x
14.148	CR (7)	Y	1	4 p_x
13.591	CR (8)	Y	1	2 p_y
19.927	CR (9)	Y	1	3 p_y
-209.726	CR (10)	Y	1	4 p_y
26.860	CR (12)	Y	1	3 p_z
-268.875	CR (13)	Y	1	4 p_z
-24.789	CR (16)	Y	1	3 d_{yz}
-16.141	CR (18)	Y	1	3 d_{z2}
-287.292	BD (1)	Y	4- N 10	σ_{Y-N}
-167.726	BD (2)	Y	4- N 10	π_{Y-N}
-286.539	BD (1)	Y	4- N 11	σ_{Y-N}
-166.851	BD (2)	Y	4- N 11	π_{Y-N}
-12.385	BD (1)	H	6- N 10	σ_{N-H}
-12.430	BD (1)	H	9- N 11	σ_{N-H}

$Y(NH_2)_3$

Table S10: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
192.882	CR (1)	Y	1	1 s
51.555	CR (2)	Y	1	2 s
32.736	CR (6)	Y	1	3 p_x
-768.655	CR (7)	Y	1	4 p_x
32.790	CR (9)	Y	1	3 p_y
-769.036	CR (10)	Y	1	4 p_y
43.784	CR (11)	Y	1	2 p_z
26.956	CR (12)	Y	1	3 p_z
25.710	CR (13)	Y	1	4 p_z
-31.386	CR (14)	Y	1	3 d_{xy}
-31.398	CR (17)	Y	1	3 $d_{x^2-y^2}$
-366.517	BD (1)	Y	1- N 2	σ_{Y-N}
-54.507	BD (2)	Y	1- N 2	π_{Y-N}
-366.584	BD (1)	Y	1- N 3	σ_{Y-N}
-54.719	BD (2)	Y	1- N 3	π_{Y-N}
-366.411	BD (1)	Y	1- N 4	σ_{Y-N}
-54.979	BD (2)	Y	1- N 4	π_{Y-N}

Table S11: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
192.665	CR (1)	Y	1	1 s
52.023	CR (2)	Y	1	2 s
12.861	CR (5)	Y	1	2 p_x
17.851	CR (6)	Y	1	3 p_x
-225.426	CR (7)	Y	1	4 p_x
22.579	CR (8)	Y	1	2 p_y
17.821	CR (9)	Y	1	3 p_y
14.920	CR (10)	Y	1	4 p_y
24.182	CR (12)	Y	1	3 p_z
-288.590	CR (13)	Y	1	4 p_z
-23.587	CR (15)	Y	1	3 d_{xz}
-15.828	CR (18)	Y	1	3 d_{z^2}
-344.640	BD (1)	Y	1- N 2	σ_{Y-N}
-175.425	BD (2)	Y	1- N 2	π_{Y-N}
-188.766	BD (1)	Y	1- N 3	σ_{Y-N}
-127.538	BD (2)	Y	1- N 3	π_{Y-N}
-23.327	BD (1)	Y	1- N 4	σ_{Y-N}
-76.671	BD (2)	Y	1- N 4	π_{Y-N}
-13.785	BD (1)	N	2- H 5	σ_{N-H}
-20.617	RY (1)	Y	1	-
23.348	RY (39)	Y	1	5 pd

Table S12: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
192.665	CR (1)	Y	1	1 s
52.024	CR (2)	Y	1	2 s
22.567	CR (5)	Y	1	2 p_x
17.814	CR (6)	Y	1	3 p_x
14.902	CR (7)	Y	1	4 p_x
12.852	CR (8)	Y	1	2 p_y
17.819	CR (9)	Y	1	3 p_y
-224.927	CR (10)	Y	1	4 p_y
24.122	CR (12)	Y	1	3 p_z
-288.029	CR (13)	Y	1	4 p_z
-23.556	CR (16)	Y	1	3 d_{yz}
-15.823	CR (18)	Y	1	3 d_{z^2}
-26.250	BD (1)	Y	1- N 2	σ_{Y-N}
-76.113	BD (2)	Y	1- N 2	π_{Y-N}
-182.191	BD (1)	Y	1- N 3	σ_{Y-N}
-125.509	BD (2)	Y	1- N 3	π_{Y-N}
-347.521	BD (1)	Y	1- N 4	σ_{Y-N}
-178.028	BD (2)	Y	1- N 4	π_{Y-N}
-13.824	BD (1)	N	4- H 10	σ_{N-H}
-20.590	RY (1)	Y	1	4 d_{z^2}
20.121	RY (39)	Y	1	5 pd

YCl_3

Table S13: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
226.172	CR(1)	Y	1	1 s
24.412	CR(6)	Y	1	3 p_x
-500.003	CR(7)	Y	1	4 p_x
24.670	CR(9)	Y	1	3 p_y
-500.973	CR(10)	Y	1	4 p_y
25.548	CR(11)	Y	1	2 p_z
-31.004	CR(14)	Y	1	3 d_{xy}
-31.179	CR(17)	Y	1	3 $d_{x^2-y^2}$
-40.442	LP(1)	Cl	2	n_{p_1}
-7.330	LP(2)	Cl	2	n_{p_2}
-38.844	LP(3)	Cl	2	n_{p_3}
-40.550	LP(1)	Cl	3	n_{p_1}
-7.309	LP(2)	Cl	3	n_{p_2}
-41.679	LP(3)	Cl	3	n_{p_3}
-40.574	LP(1)	Cl	4	n_{p_1}
-7.455	LP(2)	Cl	4	n_{p_2}
-41.770	LP(3)	Cl	4	n_{p_3}
-425.018	BD(1)	Y	1-Cl 2	σ_{Y-Cl}
-425.224	BD(1)	Y	1-Cl 3	σ_{Y-Cl}
-424.866	BD(1)	Y	1-Cl 4	σ_{Y-Cl}

Table S14: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
226.158	CR(1)	Y	1	1 s
18.157	CR(2)	Y	1	2 s
-21.130	CR(4)	Y	1	4 s
-238.895	CR(7)	Y	1	4 p_x
18.990	CR(8)	Y	1	2 p_y
15.958	CR(9)	Y	1	3 p_y
15.834	CR(10)	Y	1	4 p_y
17.275	CR(12)	Y	1	3 p_z
-185.074	CR(13)	Y	1	4 p_z
-14.743	CR(15)	Y	1	3 d_{xz}
-12.064	CR(18)	Y	1	3 d_{z^2}
-37.765	LP(1)	Cl	2	n_{p_1}
-16.535	LP(2)	Cl	2	n_{p_2}
-78.784	LP(3)	Cl	2	n_{p_3}
-40.189	LP(1)	Cl	3	n_{p_1}
-17.674	LP(2)	Cl	3	n_{p_2}
-99.962	LP(3)	Cl	3	n_{p_3}
-317.128	BD(1)	Y	1-Cl 2	σ_{Y-Cl}
-337.568	BD(1)	Y	1-Cl 3	σ_{Y-Cl}
-15.921	RY(32)	Y	1	5 spd

Table S15: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
226.165	CR(1)	Y	1	1 s
18.162	CR(2)	Y	1	2 s
-20.879	CR(4)	Y	1	4 s
18.924	CR(5)	Y	1	2 p_x
15.898	CR(6)	Y	1	3 p_x
15.798	CR(7)	Y	1	4 p_x
-234.422	CR(10)	Y	1	4 p_y
16.939	CR(12)	Y	1	3 p_z
-180.931	CR(13)	Y	1	4 p_z
-14.614	CR(16)	Y	1	3 d_{yz}
-12.005	CR(18)	Y	1	3 d_{z^2}
-14.074	LP(1)	Cl	2	n_{p_1}
-29.334	LP(3)	Cl	2	n_{p_3}
-11.688	LP(1)	Cl	3	n_{p_1}
-24.618	LP(3)	Cl	3	n_{p_3}
-51.604	LP(1)	Cl	4	n_{p_1}
-23.530	LP(2)	Cl	4	n_{p_2}
-125.334	LP(3)	Cl	4	n_{p_3}
-118.533	BD(1)	Y	1-Cl 2	σ_{Y-Cl}
-98.253	BD(1)	Y	1-Cl 3	σ_{Y-Cl}
-434.180	BD(1)	Y	1-Cl 4	σ_{Y-Cl}
-17.349	RY(32)	Y	1	5 spd

$Y(OH)_3$

Table S16: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
184.920	CR (1)	Y	1	1 s
59.889	CR (2)	Y	1	2 s
26.254	CR (5)	Y	1	2 p_x
54.522	CR (6)	Y	1	3 p_x
-516.162	CR (7)	Y	1	4 p_x
26.219	CR (8)	Y	1	2 p_y
54.593	CR (9)	Y	1	3 p_y
-516.835	CR (10)	Y	1	4 p_y
44.541	CR (11)	Y	1	2 p_z
23.942	CR (12)	Y	1	3 p_z
18.725	CR (13)	Y	1	4 p_z
-25.412	CR (14)	Y	1	3 d_{xy}
-25.434	CR (17)	Y	1	3 $d_{x^2-y^2}$
20.886	LP (1)	O	2	n_{p_1}
-37.492	LP (2)	O	2	n_{p_2}
20.920	LP (1)	O	3	n_{p_1}
-35.011	LP (2)	O	3	n_{p_2}
20.970	LP (1)	O	4	n_{p_1}
-37.359	LP (2)	O	4	n_{p_2}
-175.893	BD (1)	Y	1- O 2	σ_{Y-O}
-177.797	BD (1)	Y	1- O 3	σ_{Y-O}
-175.694	BD (1)	Y	1- O 4	σ_{Y-O}
-28.619	BD (1)	O	2- H 5	σ_{O-H}
-28.464	BD (1)	O	2- H 6	σ_{O-H}
-28.487	BD (1)	O	2- H 7	σ_{O-H}
-15.784	RY (22)	Y	1	5 p_z

Table S17: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
184.887	CR (1)	Y	1	1 s
59.960	CR (2)	Y	1	2 s
7.165	CR (3)	Y	1	3 s
16.686	CR (5)	Y	1	2 p_x
23.228	CR (6)	Y	1	3 p_x
-155.818	CR (7)	Y	1	4 p_x
23.742	CR (8)	Y	1	2 p_y
18.583	CR (9)	Y	1	3 p_y
12.293	CR (10)	Y	1	4 p_y
31.453	CR (12)	Y	1	3 p_z
-291.369	CR (13)	Y	1	4 p_z
-14.892	CR (15)	Y	1	3 d_{xz}
-11.173	CR (18)	Y	1	3 d_{z^2}
4.172	LP (1)	O	2	n_{p_1}
-6.312	LP (2)	O	2	n_{p_2}
-9.493	LP (1)	O	3	n_{p_1}
-36.298	LP (2)	O	3	n_{p_2}
-22.142	LP (1)	O	4	n_{p_1}
-84.772	LP (2)	O	4	n_{p_2}
-11.543	BD (1)	Y	1- O 2	σ_{Y-O}
-89.668	BD (1)	Y	1- O 3	σ_{Y-O}
-165.656	BD (1)	Y	1- O 4	σ_{Y-O}
-18.212	BD (1)	O	3- H 6	σ_{O-H}
-33.779	BD (1)	O	4- H 7	σ_{O-H}
-5.968	LV (3)	Y	1	-
-9.534	RY (19)	Y	1	5 pd
-11.678	RY (23)	Y	1	5 p_z
8.067	RY (25)	Y	1	5 s
-6.707	RY (49)	Y	1	-

Table S18: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
184.887	CR (1)	Y	1	1 s
59.961	CR (2)	Y	1	2 s
7.173	CR (3)	Y	1	3 s
23.722	CR (5)	Y	1	2 p_x
18.589	CR (6)	Y	1	3 p_x
12.227	CR (7)	Y	1	4 p_x
16.665	CR (8)	Y	1	2 p_y
23.215	CR (9)	Y	1	3 p_y
-155.372	CR (10)	Y	1	4 p_y
31.373	CR (12)	Y	1	3 p_z
-290.516	CR (13)	Y	1	4 p_z
-14.855	CR (16)	Y	1	3 d_{yz}
-11.170	CR (18)	Y	1	3 d_{z^2}
-22.460	LP (1)	O	2	n_{p_1}
-84.892	LP (2)	O	2	n_{p_2}
-8.791	LP (1)	O	3	n_{p_1}
-37.028	LP (2)	O	3	n_{p_2}
3.887	LP (1)	O	4	n_{p_1}
-5.362	LP (2)	O	4	n_{p_2}
-165.744	BD (1)	Y	1- O 2	σ_{Y-O}
-89.111	BD (1)	Y	1- O 3	σ_{Y-O}
-11.406	BD (1)	Y	1- O 4	σ_{Y-O}
-33.930	BD (1)	O	2- H 5	σ_{O-H}
-18.051	BD (1)	O	3- H 6	σ_{O-H}
-5.963	LV (3)	Y	1	-
-7.392	RY (13)	Y	1	5 sd
-12.905	RY (23)	Y	1	5 p_z
8.003	RY (25)	Y	1	5 s

$Y(OCH_3)_3$

Table S19: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
177.811	CR(1)	Y	1	1 s
67.045	CR(2)	Y	1	2 s
20.604	CR(5)	Y	1	2 p_x
38.854	CR(6)	Y	1	3 p_x
-489.942	CR(7)	Y	1	4 p_x
20.562	CR(8)	Y	1	2 p_y
38.871	CR(9)	Y	1	3 p_y
-490.235	CR(10)	Y	1	4 p_y
37.580	CR(11)	Y	1	2 p_z
22.239	CR(12)	Y	1	3 p_z
17.864	CR(13)	Y	1	4 p_z
-26.790	CR(14)	Y	1	3 d_{xy}
-26.725	CR(17)	Y	1	3 $d_{x^2-y^2}$
22.884	LP(1)	O	2	n_{p_1}
-39.681	LP(2)	O	2	n_{p_2}
22.974	LP(1)	O	3	n_{p_1}
-39.961	LP(2)	O	3	n_{p_2}
23.062	LP(1)	O	4	n_{p_1}
-39.522	LP(2)	O	4	n_{p_2}
-174.892	BD(1)	Y	1-O 2	σ_{Y-O}
-175.066	BD(1)	Y	1-O 3	σ_{Y-O}
-174.845	BD(1)	Y	1-O 4	σ_{Y-O}
-23.755	BD(1)	O	2-C 5	σ_{O-C}
-23.726	BD(1)	O	3-C 7	σ_{O-C}
-23.894	BD(1)	O	4-C 6	σ_{O-C}

Table S20: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
177.736	CR(1)	Y	1	1 s
67.199	CR(2)	Y	1	2 s
6.965	CR(3)	Y	1	3 s
15.422	CR(5)	Y	1	2 p_x
14.181	CR(6)	Y	1	3 p_x
-110.146	CR(7)	Y	1	4 p_x
21.324	CR(8)	Y	1	2 p_y
17.211	CR(9)	Y	1	3 p_y
25.194	CR(12)	Y	1	3 p_z
-303.004	CR(13)	Y	1	4 p_z
-14.814	CR(15)	Y	1	3 d_{xz}
-11.392	CR(18)	Y	1	3 d_{z2}
-27.546	LP(2)	O	2	n_{p_1}
-25.859	LP(1)	O	3	n_{p_1}
-97.162	LP(2)	O	3	n_{p_2}
-25.493	LP(2)	O	4	n_{p_1}
-47.064	BD(1)	Y	1-O 2	σ_{Y-O}
-176.700	BD(1)	Y	1-O 3	σ_{Y-O}
-40.943	BD(1)	Y	1-O 4	σ_{Y-O}
-8.057	BD(1)	O	2-C 5	σ_{O-C}
-30.020	BD(1)	O	3-C 7	σ_{O-C}
-6.977	BD(1)	O	4-C 6	σ_{O-C}
-17.294	BD(1)	C	7-H 15	σ_{C-H}
-9.265	BD(1)	C	7-H 16	σ_{C-H}

Table S21: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
177.736	CR(1)	Y	1	1 s
67.200	CR(2)	Y	1	2 s
6.969	CR(3)	Y	1	3 s
21.308	CR(5)	Y	1	2 p_x
17.205	CR(6)	Y	1	3 p_x
15.415	CR(8)	Y	1	2 p_y
14.157	CR(9)	Y	1	3 p_y
-109.844	CR(10)	Y	1	4 p_y
25.152	CR(12)	Y	1	3 p_z
-302.287	CR(13)	Y	1	4 p_z
-14.807	CR(16)	Y	1	3 d_{yz}
-11.377	CR(18)	Y	1	3 d_{z2}
-16.431	LP(1)	O	2	n_{p_1}
-71.851	LP(2)	O	2	n_{p_2}
4.145	LP(1)	O	3	n_{p_1}
-20.417	LP(1)	O	4	n_{p_1}
-73.657	LP(2)	O	4	n_{p_2}
-129.358	BD(1)	Y	1-O 2	σ_{Y-O}
-135.121	BD(1)	Y	1-O 4	σ_{Y-O}
-21.975	BD(1)	O	2-C 5	σ_{O-C}
-23.127	BD(1)	O	4-C 6	σ_{O-C}
-7.431	BD(1)	C	5-H 8	σ_{C-H}
-11.676	BD(1)	C	5-H 10	σ_{C-H}
-12.883	BD(1)	C	6-H 11	σ_{C-H}

$Y(N(CH_3)_2)_3$

Table S22: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
226.803	CR (1)	Y	1	1 s
22.084	CR (6)	Y	1	3 p_x
-616.330	CR (7)	Y	1	4 p_x
22.090	CR (9)	Y	1	3 p_y
-616.355	CR (10)	Y	1	4 p_y
34.778	CR (11)	Y	1	2 p_z
24.262	CR (12)	Y	1	3 p_z
22.188	CR (13)	Y	1	4 p_z
-22.962	CR (14)	Y	1	3 d_{xy}
-23.034	CR (17)	Y	1	3 $d_{x^2-y^2}$
-335.299	BD (1)	Y	1-N 2	σ_{Y-N}
-77.033	BD (2)	Y	1-N 2	π_{Y-N}
-335.021	BD (1)	Y	1-N 3	σ_{Y-N}
-76.181	BD (2)	Y	1-N 3	π_{Y-N}
-335.049	BD (1)	Y	1-N 4	σ_{Y-N}
-76.858	BD (2)	Y	1-N 4	π_{Y-N}

Table S23: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
226.789	CR (1)	Y	1	1 s
18.435	CR (2)	Y	1	2 s
-188.492	CR (7)	Y	1	4 p_x
20.511	CR (8)	Y	1	2 p_y
17.947	CR (9)	Y	1	3 p_y
12.871	CR (10)	Y	1	4 p_y
18.985	CR (12)	Y	1	3 p_z
-303.102	CR (13)	Y	1	4 p_z
-20.269	CR (15)	Y	1	3 d_{xz}
-44.831	BD (1)	Y	1-N 2	σ_{Y-N}
-120.979	BD (2)	Y	1-N 2	π_{Y-N}
-385.845	BD (1)	Y	1-N 3	σ_{Y-N}
-253.810	BD (2)	Y	1-N 3	π_{Y-N}
-168.949	BD (1)	Y	1-N 4	σ_{Y-N}
-171.450	BD (2)	Y	1-N 4	π_{Y-N}
-34.782	RY (4)	Y	1	4 d_{z^2}

Table S24: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
226.789	CR (1)	Y	1	1 s
18.435	CR (2)	Y	1	2 s
20.523	CR (5)	Y	1	2 p_x
17.945	CR (6)	Y	1	3 p_x
12.894	CR (7)	Y	1	4 p_x
-187.586	CR (10)	Y	1	4 p_y
18.966	CR (12)	Y	1	3 p_z
-303.064	CR (13)	Y	1	4 p_z
-20.256	CR (16)	Y	1	3 d_{yz}
-355.017	BD (1)	Y	1-N 2	σ_{Y-N}
-245.303	BD (2)	Y	1-N 2	π_{Y-N}
-106.676	BD (2)	Y	1-N 3	π_{Y-N}
-230.457	BD (1)	Y	1-N 4	σ_{Y-N}
-193.791	BD (2)	Y	1-N 4	π_{Y-N}
-34.675	RY (4)	Y	1	4 d_{z^2}

$Y(CH_3)_3$(thf)

Table S25: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
224.684	CR (1)	Y	1	1 s
-573.522	CR (10)	Y	1	4 p_y
-578.969	CR (13)	Y	1	4 p_x
-709.568	BD (1)	Y	1-C 2	σ_{Y-C}
-709.971	BD (1)	Y	1-C 3	σ_{Y-C}
-699.093	BD (1)	Y	1-C 4	σ_{Y-C}

Table S26: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
224.701	CR (1)	Y	1	1 s
20.267	CR (2)	Y	1	2 s
-402.442	CR (7)	Y	1	4 p_z
-273.179	CR (10)	Y	1	4 p_y
-41.874	CR (13)	Y	1	4 p_x
-72.042	LP (2)	O	26	σ_{Y-O}
-273.237	BD (1)	Y	1-C 2	σ_{Y-C}
-768.020	BD (1)	Y	1-C 3	σ_{Y-C}
-210.446	BD (1)	Y	1-C 4	σ_{Y-C}
-10.130	BD (1)	C	3-H 12	σ_{Y-H}
-11.864	BD (1)	C	3-H 14	σ_{Y-H}
23.227	RY (10)	Y	1	5 spd
-19.635	RY (15)	Y	1	5 spd
-51.562	RY (29)	Y	1	5 spd
67.646	RY (30)	Y	1	5 sp
64.932	RY (31)	Y	1	5 sp
-63.882	RY (40)	Y	1	5 s
-24.258	RY (2)	O	26	pd

Table S27: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
224.697	CR (1)	Y	1	1 s
20.267	CR (2)	Y	1	2 s
-374.444	CR (7)	Y	1	4 p_z
-45.387	CR (10)	Y	1	4 p_y
-275.278	CR (13)	Y	1	4 p_x
-80.219	LP (2)	O	26	σ_{Y-O}
-556.841	BD (1)	Y	1-C 2	σ_{Y-C}
-55.925	BD (1)	Y	1-C 3	σ_{Y-C}
-610.877	BD (1)	Y	1-C 4	σ_{Y-C}
-10.237	BD (1)	C	4-H 15	σ_{Y-H}
-12.099	BD (1)	C	4-H 17	σ_{Y-H}
22.382	RY (10)	Y	1	5 spd
-20.492	RY (15)	Y	1	5 spd
-42.646	RY (29)	Y	1	5 spd
67.546	RY (30)	Y	1	5 sp
73.627	RY (31)	Y	1	5 sp
-67.590	RY (40)	Y	1	5 s
-23.843	RY (2)	O	26	pd

cis-$Y(CH_3)_3(thf)_2$

Table S28: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
226.960	CR (1)	Y	1	1 s
-511.975	CR (7)	Y	1	4 p_x
-545.372	CR (13)	Y	1	4 p_y
-543.278	BD (1)	Y	1-C 4	σ_{Y-C}
-643.204	BD (1)	Y	1-C 5	σ_{Y-C}
-663.936	BD (1)	Y	1-C 6	σ_{Y-C}

Table S29: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
226.965	CR (1)	Y	1	1 s
10.860	CR (7)	Y	1	4 p_x
-413.360	CR (10)	Y	1	4 p_z
-333.934	CR (13)	Y	1	4 p_y
-35.578	LP (2)	O	3	σ_{Y-O}
-157.444	BD (1)	Y	1-C 4	σ_{Y-C}
-465.953	BD (1)	Y	1-C 5	σ_{Y-C}
-614.283	BD (1)	Y	1-C 6	σ_{Y-C}
-9.552	BD (1)	C	6-H 22	σ_{Y-H}
-19.781	RY (24)	Y	1	5 pd
22.642	RY (32)	Y	1	5 spd
-29.404	RY (37)	Y	1	5 p
38.655	RY (38)	Y	1	5 s
-25.742	RY (42)	Y	1	5 d

Table S30: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
226.967	CR (1)	Y	1	1 s
18.070	CR (2)	Y	1	2 s
-266.943	CR (7)	Y	1	4 p_x
-366.647	CR (10)	Y	1	4 p_z
18.520	CR (12)	Y	1	3 p_y
11.626	CR (13)	Y	1	4 p_y
-22.013	CR (14)	Y	1	3 d_{xy}
-30.176	LP (2)	O	2	σ_{Y-O}
-40.212	LP (2)	O	3	σ_{Y-O}
-629.915	BD (1)	Y	1-C 4	σ_{Y-C}
-289.064	BD (1)	Y	1-C 5	σ_{Y-C}
-145.186	BD (1)	Y	1-C 6	σ_{Y-C}
-11.485	BD (1)	C	4-H 15	σ_{Y-H}
-19.428	RY (17)	Y	1	5 spd
17.340	RY (19)	Y	1	5 spd
-21.091	RY (24)	Y	1	5 pd
24.520	RY (32)	Y	1	5 spd
-38.259	RY (37)	Y	1	5 p
17.693	RY (42)	Y	1	5 d

trans-$Y(CH_3)_3(thf)_2$

Table S31: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
228.289	CR (1)	Y	1	1 s
-735.731	CR (10)	Y	1	4 p_y
-736.451	CR (13)	Y	1	4 p_x
-711.298	BD (1)	Y	1-C 4	σ_{Y-C}
-698.626	BD (1)	Y	1-C 5	σ_{Y-C}
-702.882	BD (1)	Y	1-C 6	σ_{Y-C}

Table S32: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
228.294	CR (1)	Y	1	1 s
16.868	CR (2)	Y	1	2 s
-271.295	CR (7)	Y	1	4 p_z
-288.107	CR (10)	Y	1	4 p_y
17.041	CR (12)	Y	1	3 p_x
-22.886	CR (17)	Y	1	3 $d_{x^2-y^2}$
-41.299	LP (2)	O	2	σ_{Y-O}
-17.119	LP (1)	O	3	n_p
-35.984	LP (2)	O	3	σ_{Y-O}
-44.124	BD (1)	Y	1-C 4	σ_{Y-C}
-555.399	BD (1)	Y	1-C 5	σ_{Y-C}
-305.499	BD (1)	Y	1-C 6	σ_{Y-C}
-14.871	BD (1)	C	5-H 22	σ_{C-H}
-12.336	BD (1)	C	5-H 23	σ_{C-H}

Table S33: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
228.293	CR (1)	Y	1	1 s
16.867	CR (2)	Y	1	2 s
-274.031	CR (7)	Y	1	4 p_z
17.397	CR (9)	Y	1	3 p_y
-285.030	CR (13)	Y	1	4 p_x
-18.195	CR (18)	Y	1	3 d_{z2}
-48.910	LP (2)	O	2	σ_{Y-O}
-45.464	LP (2)	O	3	σ_{Y-O}
-562.771	BD (1)	Y	1-C 4	σ_{Y-C}
-40.169	BD (1)	Y	1-C 5	σ_{Y-C}
-294.535	BD (1)	Y	1-C 6	σ_{Y-C}
-9.423	BD (1)	C	4-H 15	σ_{C-H}
-13.548	BD (1)	C	4-H 17	σ_{C-H}

$Y(CH_3)_3$ - $\theta = 180^\circ$

Table S34: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
223.543	CR (1)	Y	1	1 s
-484.621	CR (7)	Y	1	4 p_x
-486.151	CR (10)	Y	1	4 p_y
-735.701	BD (1)	Y	1-C 2	σ_{Y-C}
-736.739	BD (1)	Y	1-C 3	σ_{Y-C}
-736.300	BD (1)	Y	1-C 4	σ_{Y-C}

Table S35: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
223.567	CR (1)	Y	1	1 s
20.982	CR (2)	Y	1	2 s
-32.884	CR (4)	Y	1	4 s
-234.564	CR (7)	Y	1	4 p_x
-179.558	CR (13)	Y	1	4 p_z
-19.207	CR (15)	Y	1	3 d_{xz}
-812.857	BD (1)	Y	1-C 2	σ_{Y-C}
-182.482	BD (1)	Y	1-C 3	σ_{Y-C}
-422.007	BD (1)	Y	1-C 4	σ_{Y-C}
-10.374	BD (1)	C	2-H 5	σ_{C-H}
-21.793	BD (1)	C	2-H 7	σ_{C-H}
-10.696	BD (1)	C	4-H 12	σ_{C-H}
54.749	RY (13)	Y	1	5 spd
-27.743	RY (14)	Y	1	5 spd
17.504	RY (15)	Y	1	5 spd
21.605	RY (16)	Y	1	5 spd
-24.353	RY (20)	Y	1	5 spd
-19.368	RY (21)	Y	1	5 spd
30.279	RY (23)	Y	1	5 spd
-206.831	RY (24)	Y	1	5 s
23.596	RY (26)	Y	1	5 spd
91.509	RY (40)	Y	1	5 spd
31.686	RY (42)	Y	1	5 spd

Table S36: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
223.567	CR (1)	Y	1	1 s
20.983	CR (2)	Y	1	2 s
-32.732	CR (4)	Y	1	4 s
-234.228	CR (10)	Y	1	4 p_y
-178.142	CR (13)	Y	1	4 p_z
-19.087	CR (16)	Y	1	3 d_{yz}
-132.165	BD (1)	Y	1-C 2	σ_{Y-C}
-761.019	BD (1)	Y	1-C 3	σ_{Y-C}
-521.913	BD (1)	Y	1-C 4	σ_{Y-C}
-18.668	BD (1)	C	3-H 9	σ_{C-H}
-7.344	BD (1)	C	3-H 10	σ_{C-H}
-16.576	BD (1)	C	4-H 12	σ_{C-H}
-7.701	BD (1)	C	4-H 13	σ_{C-H}
54.586	RY (13)	Y	1	5 spd
-27.749	RY (14)	Y	1	5 spd
17.573	RY (15)	Y	1	5 spd
22.383	RY (16)	Y	1	5 spd
-28.557	RY (20)	Y	1	5 spd
30.903	RY (23)	Y	1	5 spd
-197.364	RY (24)	Y	1	5 s
37.030	RY (26)	Y	1	5 spd
56.982	RY (40)	Y	1	5 spd
33.789	RY (42)	Y	1	5 spd

5.2 Reported Organoyttrium Compounds

$Y(CH(SiMe_3)_2)_3$

Table S37: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
229.186	CR (1)	Y	1	1 s
-57.806	CR (5)	Y	1	2 p_x
-34.462	CR (6)	Y	1	3 p_x
-390.941	CR (7)	Y	1	4 p_x
-57.765	CR (8)	Y	1	2 p_y
-34.292	CR (9)	Y	1	3 p_y
-392.820	CR (10)	Y	1	4 p_y
-34.491	CR (11)	Y	1	2 p_z
-27.524	CR (14)	Y	1	3 d_{xy}
-27.557	CR (17)	Y	1	3 $d_{x^2-y^2}$
-565.534	BD (1)	Y	1-C 2	σ_{Y-C}
-566.398	BD (1)	Y	1-C 3	σ_{Y-C}
-566.942	BD (1)	Y	1-C 4	σ_{Y-C}

Table S38: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
229.125	CR (1)	Y	1	1 s
-17.788	CR (4)	Y	1	4 s
-58.458	CR (5)	Y	1	2 p_x
-49.746	CR (6)	Y	1	3 p_x
-196.553	CR (7)	Y	1	4 p_x
-33.926	CR (8)	Y	1	2 p_y
-41.072	CR (11)	Y	1	2 p_z
-124.503	CR (13)	Y	1	4 p_z
-17.282	CR (15)	Y	1	3 d_{xz}
-169.801	BD (1)	Y	1-C 2	σ_{Y-C}
-277.979	BD (1)	Y	1-C 3	σ_{Y-C}
-651.561	BD (1)	Y	1-C 4	σ_{Y-C}
-16.996	BD (1)	C	4-Si 25	σ_{C-Si}
-18.516	BD (1)	C	4-Si 26	σ_{C-Si}
30.522	RY (29)	Y	1	5 s
-36.557	RY (35)	Y	1	5 p
17.663	RY (36)	Y	1	5 sd
-19.854	RY (37)	Y	1	5 sp

Table S39: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
229.125	CR (1)	Y	1	1 s
-17.724	CR (4)	Y	1	4 s
-33.803	CR (5)	Y	1	2 p_x
-58.293	CR (8)	Y	1	2 p_y
-49.733	CR (9)	Y	1	3 p_y
-197.236	CR (10)	Y	1	4 p_y
-40.972	CR (11)	Y	1	2 p_z
-123.308	CR (13)	Y	1	4 p_z
-17.192	CR (16)	Y	1	3 d_{yz}
-562.055	BD (1)	Y	1-C 2	σ_{Y-C}
-454.440	BD (1)	Y	1-C 3	σ_{Y-C}
-81.293	BD (1)	Y	1-C 4	σ_{Y-C}
-12.896	BD (1)	C	2-Si 23	σ_{C-Si}
-21.059	BD (1)	C	2-Si 24	σ_{C-Si}
-14.790	BD (1)	C	3-Si 28	σ_{C-Si}
30.305	RY (29)	Y	1	5 s
-36.128	RY (35)	Y	1	5 p
17.275	RY (36)	Y	1	5 sd
-19.781	RY (37)	Y	1	5 sp

$Y(N(SiMe_3)_2)_3$

Table S40: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
229.222	CR (1)	Y	1	1 s
-37.009	CR (5)	Y	1	2 p_x
-23.305	CR (6)	Y	1	3 p_x
-374.517	CR (7)	Y	1	4 p_x
-36.661	CR (8)	Y	1	2 p_y
-23.402	CR (9)	Y	1	3 p_y
-374.421	CR (10)	Y	1	4 p_y
-24.649	CR (14)	Y	1	3 d_{xy}
-24.620	CR (17)	Y	1	3 $d_{x^2-y^2}$
-343.984	LP (1)	N	2	σ_{Y-N}
-33.515	LP (2)	N	2	π_{Y-N}
-322.968	LP (1)	N	3	σ_{Y-N}
-33.837	LP (2)	N	3	π_{Y-N}
-347.424	LP (1)	N	4	σ_{Y-N}
-35.327	LP (2)	N	4	π_{Y-N}

Table S41: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
229.218	CR (1)	Y	1	1 s
15.872	CR (2)	Y	1	2 s
-11.165	CR (4)	Y	1	4 s
-22.672	CR (5)	Y	1	2 p_x
8.334	CR (7)	Y	1	4 p_x
-50.384	CR (8)	Y	1	2 p_y
-50.803	CR (9)	Y	1	3 p_y
-185.652	CR (10)	Y	1	4 p_y
-32.911	CR (11)	Y	1	2 p_z
-11.370	CR (12)	Y	1	3 p_z
-105.701	CR (13)	Y	1	4 p_z
-14.079	CR (16)	Y	1	3 d_{yz}
-67.086	LP (1)	N	2	σ_{Y-N}
-30.602	LP (2)	N	2	π_{Y-N}
-353.435	LP (1)	N	3	σ_{Y-N}
-82.213	LP (2)	N	3	π_{Y-N}
-156.000	LP (1)	N	4	σ_{Y-N}
-47.132	LP (2)	N	4	π_{Y-N}
-15.782	BD (1)	N	3-Si 9	σ_{N-Si}
-6.937	BD (1)	N	3-Si 10	σ_{N-Si}
-11.065	BD (1)	C	25-H 72	σ_{C-H}

Table S42: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
229.218	CR (1)	Y	1	1 s
15.869	CR (2)	Y	1	2 s
-10.938	CR (4)	Y	1	4 s
-51.553	CR (5)	Y	1	2 p_x
-51.908	CR (6)	Y	1	3 p_x
-184.623	CR (7)	Y	1	4 p_x
-23.368	CR (8)	Y	1	2 p_y
8.622	CR (10)	Y	1	4 p_y
-33.106	CR (11)	Y	1	2 p_z
-11.645	CR (12)	Y	1	3 p_z
-100.918	CR (13)	Y	1	4 p_z
-13.917	CR (15)	Y	1	3 d_{xz}
-316.263	LP (1)	N	2	σ_{Y-N}
-67.918	LP (2)	N	2	π_{Y-N}
-28.216	LP (1)	N	3	σ_{Y-N}
-25.024	LP (2)	N	3	π_{Y-N}
-230.779	LP (1)	N	4	σ_{Y-N}
-59.530	LP (2)	N	4	π_{Y-N}
-12.727	BD (1)	N	2-Si 5	σ_{N-Si}
-8.647	BD (1)	N	2-Si 6	σ_{N-Si}
-9.523	BD (1)	N	4-Si 8	σ_{N-Si}

Y(O-2,6-*t*-Bu$_2$C$_6$H$_3$)$_3$

Table S43: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
231.551	CR (1)	Y	1	1 s
13.702	CR (2)	Y	1	2 s
-331.490	CR (7)	Y	1	4 p_x
-427.004	CR (10)	Y	1	4 p_y
15.350	CR (12)	Y	1	3 p_z
13.607	CR (13)	Y	1	4 p_z
-22.410	CR (14)	Y	1	3 d_{xy}
-21.278	CR (17)	Y	1	3 $d_{x^2-y^2}$
-159.470	LP (1)	O	2	σ_{Y-O}
-15.005	LP (2)	O	2	np_1
-16.934	LP (3)	O	2	np_2
-116.777	LP (1)	O	3	σ_{Y-O}
-69.824	LP (2)	O	3	np_1
-6.908	LP (3)	O	3	np_2
-123.052	LP (1)	O	4	σ_{Y-O}
-65.234	LP (2)	O	4	np_1
-4.992	LP (3)	O	4	np_2
-30.638	BD (1)	O	2-C 11	σ_{O-C}
-27.534	BD (1)	O	3-C 5	σ_{O-C}
-28.021	BD (1)	O	4-C 17	σ_{O-C}

Table S44: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
231.553	CR (1)	Y	1	1 s
13.711	CR (2)	Y	1	2 s
-21.050	CR (5)	Y	1	2 p_x
-27.311	CR (6)	Y	1	3 p_x
-62.265	CR (7)	Y	1	4 p_x
11.270	CR (9)	Y	1	3 p_y
12.935	CR (10)	Y	1	4 p_y
-27.533	CR (11)	Y	1	2 p_z
-250.165	CR (13)	Y	1	4 p_z
-11.467	CR (15)	Y	1	3 d_{xz}
-147.103	LP (1)	O	2	σ_{Y-O}
-56.781	LP (2)	O	2	np_1
-56.998	LP (3)	O	2	np_2
-57.059	LP (1)	O	3	σ_{Y-O}
-33.307	LP (2)	O	3	np_1
-14.887	LP (3)	O	3	np_2
-39.226	LP (1)	O	4	σ_{Y-O}
-22.136	LP (2)	O	4	np_1
-12.818	LP (3)	O	4	np_2
-36.565	BD (1)	O	2-C 11	σ_{O-C}
-13.861	BD (1)	O	3-C 5	σ_{O-C}
-9.311	BD (1)	O	4-C 17	σ_{O-C}
-17.262	BD (2)	C	11-C 12	π_{C-C}
-8.578	BD (1)	C	34-H 80	σ_{C-H}
-10.693	BD (1)	C	40-H 92	σ_{C-H}
-8.222	BD (1)	C	40-H 94	σ_{C-H}
8.739	RY (34)	Y	1	5 s
-11.008	RY (42)	Y	1	5 d

Table S45: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
231.549	CR (1)	Y	1	1 s
13.709	CR (2)	Y	1	2 s
7.492	CR (3)	Y	1	3 s
11.921	CR (6)	Y	1	3 p_x
12.648	CR (7)	Y	1	4 p_x
-10.295	CR (8)	Y	1	2 p_y
-25.316	CR (9)	Y	1	3 p_y
-74.462	CR (10)	Y	1	4 p_y
-24.341	CR (11)	Y	1	2 p_z
-10.847	CR (12)	Y	1	3 p_z
-181.599	CR (13)	Y	1	4 p_z
-9.135	CR (16)	Y	1	3 d_{yz}
-7.286	CR (18)	Y	1	3 d_{z2}
-79.037	LP (1)	O	3	σ_{Y-O}
-70.655	LP (2)	O	3	np_1
-27.524	LP (3)	O	3	np_2
-102.217	LP (1)	O	4	σ_{Y-O}
-81.067	LP (2)	O	4	np_1
-29.207	LP (3)	O	4	np_2
-22.081	BD (1)	O	3-C 5	σ_{O-C}
-27.605	BD (1)	O	4-C 17	σ_{O-C}
-6.935	BD (2)	C	5-C 6	π_{C-C}
-7.322	BD (1)	C	5-C 7	σ_{C-C}
-8.498	BD (1)	C	17-C 19	σ_{C-C}
-8.177	BD (1)	C	34-H 80	σ_{C-H}
-13.396	BD (1)	C	34-H 82	σ_{C-H}
-0.727	BD (1)	C	37-H 88	σ_{C-H}
-7.736	BD (1)	C	40-H 92	σ_{C-H}
-10.982	BD (1)	C	40-H 94	σ_{C-H}
12.883	RY (34)	Y	1	5 s
-8.198	RY (42)	Y	1	5 d

Y(OAr)$_3$

Table S46: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
233.252	CR (1)	Y	1	1 s
-19.065	CR (5)	Y	1	2 p_x
-349.256	CR (7)	Y	1	4 p_x
-19.779	CR (8)	Y	1	2 p_y
-329.947	CR (10)	Y	1	4 p_y
13.817	CR (12)	Y	1	3 p_z
14.076	CR (13)	Y	1	4 p_z
-21.501	CR (14)	Y	1	3 d_{xy}
-21.529	CR (17)	Y	1	3 $d_{x^2-y^2}$
-113.200	LP (1)	O	2	σ_{Y-O}
-74.780	LP (2)	O	2	np_1
-6.588	LP (3)	O	2	np_2
-128.843	LP (1)	O	3	σ_{Y-O}
-51.952	LP (2)	O	3	np_1
-18.989	LP (3)	O	3	np_2
-148.621	LP (1)	O	4	σ_{Y-O}
-27.764	LP (2)	O	4	np_1
-16.323	LP (3)	O	4	np_2
-26.516	BD (1)	O	2-C 5	σ_{O-C}
-28.166	BD (1)	O	3-C 18	σ_{O-C}
-28.927	BD (1)	O	4-C 29	σ_{O-C}
-14.290	BD (2)	C	5-C 10	π_{C-C}
-15.150	BD (2)	C	18-C 19	π_{C-C}

Table S47: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
233.256	CR (1)	Y	1	1 s
12.031	CR (2)	Y	1	2 s
-14.092	CR (5)	Y	1	2 p_x
-26.225	CR (8)	Y	1	2 p_y
-26.709	CR (9)	Y	1	3 p_y
-87.515	CR (10)	Y	1	4 p_y
-30.031	CR (11)	Y	1	2 p_z
-170.721	CR (13)	Y	1	4 p_z
-10.489	CR (16)	Y	1	3 d_{yz}
-9.693	LP (1)	O	2	σ_{Y-O}
-98.583	LP (1)	O	3	σ_{Y-O}
-54.721	LP (2)	O	3	np_1
-41.741	LP (3)	O	3	np_2
-127.407	LP (1)	O	4	σ_{Y-O}
-56.211	LP (2)	O	4	np_1
-52.559	LP (3)	O	4	np_2
-26.689	BD (1)	O	3-C 18	σ_{O-C}
-29.665	BD (1)	O	4-C 29	σ_{O-C}
-12.600	BD (1)	C	17-H 65	σ_{C-H}
-20.281	BD (1)	C	17-H 66	σ_{C-H}
-13.825	BD (2)	C	18-C 19	π_{C-C}
-16.900	BD (2)	C	29-C 30	π_{C-C}
-3.284	BD (1)	C	39-H 87	σ_{C-H}
13.038	RY (35)	Y	1	5 sd
-13.840	RY (40)	Y	1	5 sp

Table S48: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
233.254	CR (1)	Y	1	1 s
12.032	CR (2)	Y	1	2 s
7.467	CR (3)	Y	1	3 s
-24.858	CR (5)	Y	1	2 p_x
-28.182	CR (6)	Y	1	3 p_x
-108.406	CR (7)	Y	1	4 p_x
-13.215	CR (8)	Y	1	2 p_y
-9.342	CR (10)	Y	1	4 p_y
-28.255	CR (11)	Y	1	2 p_z
-9.036	CR (12)	Y	1	3 p_z
-101.171	CR (13)	Y	1	4 p_z
-9.535	CR (15)	Y	1	3 d_{xz}
-7.795	CR (18)	Y	1	3 d_{z^2}
-134.049	LP (1)	O	2	σ_{Y-O}
-103.316	LP (2)	O	2	np_1
-38.941	LP (3)	O	2	np_2
-34.165	LP (1)	O	3	σ_{Y-O}
-28.688	LP (2)	O	3	np_1
-25.597	LP (3)	O	3	np_2
-27.504	LP (1)	O	4	σ_{Y-O}
-26.146	LP (2)	O	4	np_1
-8.835	LP (3)	O	4	np_2
-37.231	BD (1)	O	2-C 5	σ_{O-C}
-10.246	BD (1)	O	3-C 18	σ_{O-C}
-9.608	BD (1)	C	5-C 6	σ_{C-C}
-8.389	BD (2)	C	5-C 10	π_{C-C}
0.705	BD (1)	C	17-H 64	σ_{C-H}
-10.439	BD (1)	C	17-H 66	σ_{C-H}
-9.205	BD (2)	C	18-C 19	π_{C-C}
-3.391	BD (1)	C	39-H 87	σ_{C-H}
-11.628	BD (1)	C	44-H 100	σ_{C-H}
-15.920	BD (1)	C	44-H 101	σ_{C-H}

$Y(CH_2(SiMe_3))_3(thf)_2$

Table S49: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
229.340	CR (1)	Y	1	1 s
-570.602	CR (7)	Y	1	4 p_x
-188.221	CR (10)	Y	1	4 p_y
-563.847	CR (13)	Y	1	4 p_z
-635.361	BD (1)	Y	1-C 12	σ_{Y-C}
-615.989	BD (1)	Y	1-C 13	σ_{Y-C}
-654.855	BD (1)	Y	1-C 14	σ_{Y-C}

Table S50: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
229.339	CR (1)	Y	1	1 s
15.789	CR (2)	Y	1	2 s
-152.176	CR (7)	Y	1	4 p_x
-15.969	CR (8)	Y	1	2 p_y
-206.377	CR (10)	Y	1	4 p_y
-166.709	CR (13)	Y	1	4 p_z
-37.795	LP (1)	O	2	σ_{Y-O}
-58.869	LP (1)	O	3	σ_{Y-O}
-49.533	BD (1)	Y	1-C 12	σ_{Y-C}
-531.241	BD (1)	Y	1-C 13	σ_{Y-C}
-253.619	BD (1)	Y	1-C 14	σ_{Y-C}
-24.042	BD (1)	C	13-Si 74	σ_{C-Si}
-16.360	BD (1)	C	14-Si 75	σ_{C-Si}

Table S51: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
229.336	CR (1)	Y	1	1 s
15.786	CR (2)	Y	1	2 s
-15.531	CR (5)	Y	1	2 p_x
-108.317	CR (7)	Y	1	4 p_x
-23.631	CR (8)	Y	1	2 p_y
-15.615	CR (9)	Y	1	3 p_y
-264.299	CR (10)	Y	1	4 p_y
-13.873	CR (11)	Y	1	2 p_z
-109.965	CR (13)	Y	1	4 p_z
-41.543	LP (1)	O	2	σ_{Y-O}
-53.092	LP (1)	O	3	σ_{Y-O}
-485.275	BD (1)	Y	1-C 12	σ_{Y-C}
-28.626	BD (1)	Y	1-C 13	σ_{Y-C}
-288.344	BD (1)	Y	1-C 14	σ_{Y-C}
-4.747	BD (1)	C	12-H 40	σ_{C-Si}
-21.962	BD (1)	C	12-Si 73	σ_{C-Si}
-17.139	RY (38)	Y	1	5 spd

$Y(N(SiMe_3)_2)_3(OPPh_3)$

Table S52: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
223.877	CR (1)	Y	1	1 s
21.331	CR (2)	Y	1	2 s
-28.943	CR (5)	Y	1	2 p_x
-49.180	CR (8)	Y	1	2 p_y
-36.886	CR (9)	Y	1	3 p_y
-285.591	CR (10)	Y	1	4 p_y
-49.158	CR (11)	Y	1	2 p_z
-36.771	CR (12)	Y	1	3 p_z
-283.368	CR (13)	Y	1	4 p_z
-20.311	CR (16)	Y	1	3 d_{yz}
-305.862	LP (1)	N	2	σ_{Y-N}
-37.264	LP (2)	N	2	π_{Y-N}
-307.191	LP (1)	N	3	σ_{Y-N}
-38.107	LP (2)	N	3	π_{Y-N}
-299.096	LP (1)	N	4	σ_{Y-N}
-38.356	LP (2)	N	4	π_{Y-N}

Table S53: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
223.924	CR (1)	Y	1	1 s
21.399	CR (2)	Y	1	2 s
-32.672	CR (5)	Y	1	2 p_x
-21.819	CR (6)	Y	1	3 p_x
-254.449	CR (7)	Y	1	4 p_x
-38.074	CR (8)	Y	1	2 p_y
-27.904	CR (9)	Y	1	3 p_y
-97.220	CR (10)	Y	1	4 p_y
-30.238	CR (11)	Y	1	2 p_z
-21.663	CR (13)	Y	1	4 p_z
-130.708	LP (1)	N	2	σ_{Y-N}
-37.891	LP (2)	N	2	π_{Y-N}
-327.383	LP (1)	N	3	σ_{Y-N}
-61.106	LP (2)	N	3	π_{Y-N}
-83.555	LP (1)	N	4	σ_{Y-N}
-27.834	LP (2)	N	4	π_{Y-N}
-75.439	LP (1)	O	116	σ_{Y-O}
-6.787	LP (2)	O	116	π_{Y-O}
-12.195	BD (1)	N	3-Si 9	σ_{Y-Si}
-8.940	BD (1)	N	3-Si 10	σ_{Y-Si}
-14.149	BD (1)	O	116- P117	σ^*_{O-P}
14.888	RY (19)	Y	1	5 spd
-13.453	RY (20)	Y	1	5 spd
66.408	RY (30)	Y	1	5 sp
19.799	RY (32)	Y	1	5 s
-24.733	RY (36)	Y	1	5 s
-68.378	RY (37)	Y	1	5 sp

Table S54: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
223.924	CR (1)	Y	1	1 s
21.399	CR (2)	Y	1	2 s
-32.654	CR (5)	Y	1	2 p_x
-21.704	CR (6)	Y	1	3 p_x
-254.075	CR (7)	Y	1	4 p_x
-30.276	CR (8)	Y	1	2 p_y
-21.659	CR (10)	Y	1	4 p_y
-38.077	CR (11)	Y	1	2 p_z
-27.837	CR (12)	Y	1	3 p_z
-96.455	CR (13)	Y	1	4 p_z
-232.293	LP (1)	N	2	σ_{Y-N}
-45.881	LP (2)	N	2	π_{Y-N}
-33.994	LP (1)	N	3	σ_{Y-N}
-24.484	LP (2)	N	3	π_{Y-N}
-275.009	LP (1)	N	4	σ_{Y-N}
-56.891	LP (2)	N	4	π_{Y-N}
-75.405	LP (1)	O	116	σ_{Y-O}
-6.589	LP (3)	O	116	π_{Y-O}
-4.192	BD (1)	N	4-Si 7	σ_{N-Si}
-0.878	BD (1)	Si	7- C 22	σ_{Si-R}
-14.161	BD (1)	O	116- P117	σ^*_{O-P}
14.868	RY (19)	Y	1	5 spd
-13.353	RY (20)	Y	1	5 spd
66.356	RY (30)	Y	1	5 sp
19.829	RY (32)	Y	1	5 s
-24.740	RY (36)	Y	1	5 s
-68.935	RY (37)	Y	1	5 sp

$Y(OAr)_3(OPMe_2Ph)$

Table S55: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
231.310	CR (1)	Y	1	1 s
14.071	CR (2)	Y	1	2 s
-19.282	CR (5)	Y	1	2 p_x
-15.004	CR (6)	Y	1	3 p_x
-230.140	CR (7)	Y	1	4 p_x
-20.950	CR (8)	Y	1	2 p_y
-15.324	CR (9)	Y	1	3 p_y
-275.137	CR (10)	Y	1	4 p_y
11.655	CR (12)	Y	1	3 p_z
-16.069	CR (14)	Y	1	3 d_{xy}
-16.339	CR (17)	Y	1	3 $d_{x^2-y^2}$
-123.941	LP (1)	O	2	σ_{Y-O}
-32.208	LP (2)	O	2	np_1
-35.570	LP (3)	O	2	np_2
-119.194	LP (1)	O	3	σ_{Y-O}
-22.762	LP (2)	O	3	np_1
-34.428	LP (3)	O	3	np_2
-130.842	LP (1)	O	4	σ_{Y-O}
-36.798	LP (2)	O	4	np_1
-16.403	LP (3)	O	4	np_2
-26.054	BD (1)	O	2-C 12	σ_{O-C}
-24.383	BD (1)	O	3-C 6	σ_{O-C}
-25.324	BD (1)	O	4-C 18	σ_{O-C}
-13.068	BD (2)	C	12-C 13	π_{C-C}
-13.714	BD (2)	C	18-C 20	π_{C-C}
-11.050	RY (35)	Y	1	5 sp

Table S56: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
231.309	CR (1)	Y	1	1 s
14.077	CR (2)	Y	1	2 s
-21.236	CR (5)	Y	1	2 p_x
-18.297	CR (6)	Y	1	3 p_x
-94.105	CR (7)	Y	1	4 p_x
-13.101	CR (8)	Y	1	2 p_y
-42.623	CR (10)	Y	1	4 p_y
-25.854	CR (11)	Y	1	2 p_z
-14.810	CR (12)	Y	1	3 p_z
-190.678	CR (13)	Y	1	4 p_z
-8.570	CR (15)	Y	1	3 d_{xz}
-117.475	LP (1)	O	2	σ_{Y-O}
-43.598	LP (2)	O	2	np_1
-37.099	LP (3)	O	2	np_2
-13.906	LP (1)	O	3	σ_{Y-O}
-13.168	LP (2)	O	3	np_1
-82.230	LP (1)	O	4	σ_{Y-O}
-40.862	LP (2)	O	4	np_1
-36.475	LP (3)	O	4	np_2
-69.395	LP (1)	O	5	σ_{Y-O}
-6.679	LP (2)	O	5	np_1
-27.627	BD (1)	O	2-C 12	σ_{O-C}
-19.986	BD (1)	O	4-C 18	σ_{O-C}
-13.487	BD (1)	O	5-P 139	σ^*_{O-P}
-11.761	BD (2)	C	12-C 13	π_{C-C}
-8.343	BD (2)	C	18-C 20	π_{C-C}
-2.424	BD (1)	C	39-H 98	σ_{C-H}
-9.786	RY (37)	Y	1	5 sp

Table S57: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
231.309	CR (1)	Y	1	1 s
14.073	CR (2)	Y	1	2 s
7.328	CR (3)	Y	1	3 s
-11.341	CR (5)	Y	1	2 p_x
-23.263	CR (7)	Y	1	4 p_x
-19.960	CR (8)	Y	1	2 p_y
-18.460	CR (9)	Y	1	3 p_y
-83.857	CR (10)	Y	1	4 p_y
-26.305	CR (11)	Y	1	2 p_z
-19.380	CR (12)	Y	1	3 p_z
-175.717	CR (13)	Y	1	4 p_z
-8.469	CR (16)	Y	1	3 d_{yz}
-8.491	CR (18)	Y	1	3 d_{z^2}
-30.701	LP (1)	O	2	σ_{Y-O}
-13.760	LP (2)	O	2	np_1
-126.941	LP (1)	O	3	σ_{Y-O}
-31.128	LP (2)	O	3	np_1
-45.948	LP (3)	O	3	np_2
-46.929	LP (1)	O	4	σ_{Y-O}
-34.164	LP (2)	O	4	np_1
-4.812	LP (3)	O	4	np_2
-71.836	LP (1)	O	5	σ_{Y-O}
-8.374	LP (3)	O	5	np_2
-6.730	BD (1)	O	2-C 12	σ_{O-C}
-28.225	BD (1)	O	3-C 6	σ_{O-C}
-11.199	BD (1)	O	4-C 18	σ_{O-C}
-12.602	BD (1)	O	5-P 139	σ^*_{O-P}
-17.031	BD (2)	C	6-C 8	π_{C-C}
-1.064	BD (1)	C	29-H 76	σ_{C-H}
-3.684	BD (1)	C	41-H 103	σ_{C-H}
-9.373	RY (37)	Y	1	5 sp

$Y(C_5H_5)_2(OPh)$

Table S58: Paramagnetic and Spin-Orbit Shielding Tensor component 1

Contribution	parent NBO label	NBO	label	Interpretation
226.826	CR (1)	Y	1	1 s
18.498	CR (2)	Y	1	2 s
7.522	CR (3)	Y	1	3 s
21.269	CR (5)	Y	1	2 p_x
16.677	CR (6)	Y	1	3 p_x
13.167	CR (7)	Y	1	4 p_x
10.051	CR (8)	Y	1	2 p_y
-167.001	CR (10)	Y	1	4 p_y
9.615	CR (11)	Y	1	2 p_z
-105.855	CR (13)	Y	1	4 p_z
-21.409	CR (16)	Y	1	3 d_{yz}
-7.807	CR (18)	Y	1	3 d_{z^2}
-42.352	LP (1)	C	8	π-interaction
-34.602	LP (1)	C	10	π-interaction
-57.532	LP (1)	C	15	π-interaction
-18.224	LP (1)	C	17	π-interaction
-10.278	BD (2)	Y	1-O 33	π_{Y-O}
13.651	BD (2)	C	4-O 33	π_{O-C}
-46.646	3C (1)	C	9-C 11- C 12	π-allylic
-32.297	3C (1)	C	13-C 14- C 16	π-allylic
-212.209	3Cn (1)	C	9-C 11- C 12	π^*-Cp
-299.937	3Cn (1)	C	13-C 14- C 16	π^*-Cp
8.468	LV (3)	Y	1	-
-29.282	LV (4)	Y	1	-
9.721	RY (4)	Y	1	5 spd
7.487	RY (8)	Y	1	5 spd
10.974	RY (12)	Y	1	5 spd
-7.990	RY (15)	Y	1	5 spd
-28.552	RY (27)	Y	1	5 sd
-13.905	RY (31)	Y	1	5 sp
19.680	RY (32)	Y	1	5 spd
-15.930	RY (33)	Y	1	5 s
15.530	RY (35)	Y	1	5 spd
15.578	RY (40)	Y	1	5 s
-13.429	RY (41)	Y	1	5 sp

Table S59: Paramagnetic and Spin-Orbit Shielding Tensor component 2

Contribution	parent NBO label	NBO	label	Interpretation
226.805	CR (1)	Y	1	1 s
18.485	CR (2)	Y	1	2 s
7.246	CR (3)	Y	1	3 s
12.653	CR (5)	Y	1	2 p_x
7.920	CR (6)	Y	1	3 p_x
-237.369	CR (7)	Y	1	4 p_x
22.387	CR (8)	Y	1	2 p_y
18.151	CR (9)	Y	1	3 p_y
14.588	CR (10)	Y	1	4 p_y
12.639	CR (12)	Y	1	3 p_z
-262.059	CR (13)	Y	1	4 p_z
-15.947	CR (15)	Y	1	3 d_{xz}
-7.374	CR (18)	Y	1	3 d_{z2}
-24.269	LP (1)	C	8	π-interaction
-14.339	LP (1)	C	10	π-interaction
45.660	LP (1)	C	15	π-interaction
9.873	LP (1)	C	17	π-interaction
-171.829	BD (1)	Y	1-O 33	σ_{Y-O}
-134.415	BD (2)	Y	1-O 33	π_{Y-O}
-10.414	BD (1)	C	2-C 4	σ_{C-C}
-10.606	BD (1)	C	4-C 5	σ_{C-C}
-32.902	BD (1)	C	4-O 33	σ_{O-C}
-20.754	BD (2)	C	4-O 33	π_{O-C}
73.487	3C (1)	C	9-C 11- C 12	π-allylic
-19.794	3C (1)	C	13-C 14- C 16	π-allylic
-55.250	3Cn (1)	C	9-C 11- C 12	π^*-Cp
-79.932	3Cn (1)	C	13-C 14- C 16	π^*-Cp
-10.173	LV (4)	Y	1	-
-8.441	RY (29)	Y	1	5 spd
9.062	RY (31)	Y	1	5 sd
16.546	RY (32)	Y	1	5 spd
45.616	RY (33)	Y	1	5 s
-8.119	RY (35)	Y	1	5 spd
-27.391	RY (39)	Y	1	5 p
-40.323	RY (40)	Y	1	5 s
9.349	RY (41)	Y	1	5 sp
8.875	RY (3)	O	33	2 p

Table S60: Paramagnetic and Spin-Orbit Shielding Tensor component 3

Contribution	parent NBO label	NBO	label	Interpretation
226.805	CR (1)	Y	1	1 s
18.474	CR (2)	Y	1	2 s
7.227	CR (3)	Y	1	3 s
27.504	CR (5)	Y	1	2 p_x
-187.061	CR (7)	Y	1	4 p_x
19.058	CR (8)	Y	1	2 p_y
28.418	CR (9)	Y	1	3 p_y
-310.422	CR (10)	Y	1	4 p_y
34.592	CR (11)	Y	1	2 p_z
19.863	CR (12)	Y	1	3 p_z
15.276	CR (13)	Y	1	4 p_z
-15.743	CR (14)	Y	1	3 d_{xy}
-19.187	CR (17)	Y	1	3 $d_{x^2-y^2}$
-16.879	LP (1)	C	8	π-interaction
-19.345	LP (1)	C	10	π-interaction
-47.817	LP (1)	C	15	π-interaction
-119.269	BD (1)	Y	1-O 33	σ_{Y-O}
-33.335	BD (2)	Y	1-O 33	π_{Y-O}
-23.673	BD (1)	C	4-O 33	σ_{O-C}
-4.256	BD (2)	C	4-O 33	π_{O-C}
-14.385	3C (1)	C	9-C 11-C 12	π-allylic
-13.074	3C (1)	C	13-C 14-C 16	π-allylic
-72.519	3Cn (1)	C	9-C 11-C 12	π^*-Cp
-111.074	3Cn (1)	C	13-C 14-C 16	π^*-Cp
6.937	RY (29)	Y	1	5 spd
-10.524	RY (31)	Y	1	5 sd
-20.220	RY (33)	Y	1	5 s
11.097	RY (35)	Y	1	5 spd
8.765	RY (39)	Y	1	5 p
18.510	RY (40)	Y	1	5 s
-7.038	RY (3)	O	33	2 p