Electronic Supplementary Information for:

" Electric field gradients of transition metal complexes from density functional theory: assessment of functionals, geometries and basis sets "

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Table S1. EFG calculations with additional functionals: V_{zz} values in au, compared to gas-phase MW data.

Comp.	M06-L	M06-HF	τ-HCTHh	VSXC	G96LYP	BB95	B1B95	BMK	O3LYP	PKZB	ωB97	ωB97X	HSEh1PBE	LC-TPSS
1	-0.666	-0.788	-0.766	-0.722	-0.729	-0.749	-0.800	-0.628	-0.734	-0.713	-0.829	-0.827	-0.764	-0.888
2	-0.277	0.110	-0.348	-0.296	-0.329	-0.313	-0.324	-0.289	-0.320	-0.305	-0.397	-0.374	-0.324	-0.433
3	-0.506	0.429	-0.485	-0.542	-0.575	-0.589	-0.405	-0.298	-0.480	-0.473	-0.314	-0.324	-0.408	-0.179
4	0.469	0.532	0.532	0.475	0.508	0.505	0.560	0.522	0.546	0.475	0.550	0.544	0.537	0.579
5	-0.675	-0.812	-0.815	-0.737	-0.763	-0.741	-0.824	-0.852	-0.767	-0.731	-0.860	-0.849	-0.811	-0.931
6	-1.057	-1.492	-1.067	-0.962	-0.906	-0.875	-1.204	-1.312	-1.032	-0.914	-1.182	-1.230	-1.142	-1.235
7	-0.377	-0.693	-0.471	-0.385	-0.388	-0.384	-0.519	-0.552	-0.443	-0.413	-0.569	-0.559	-0.505	-0.613
8	-0.268	0.088	-0.319	-0.289	-0.338	-0.326	-0.269	-0.310	-0.279	-0.309	-0.259	-0.257	-0.285	-0.278
MAE	0.133	0.333	0.096	0.137	0.130	0.143	0.083	0.088	0.110	0.134	0.076	0.082	0.086	0.087
ME	0.015	0.137	-0.025	0.008	0.000	0.010	-0.027	-0.042	0.003	0.018	-0.034	-0.036	-0.020	-0.042
MaxE	0.289	-0.646	0.268	0.326	0.359	0.373	0.188	0.196	0.264	-0.268	0.212	0.203	0.191	0.257
Slope	0.812	1.169	0.885	0.786	0.782	0.761	0.968	1.013	0.866	0.771	0.969	0.983	0.926	1.037

Table S2. EFG tensors calculated using ab initio methods: V_{zz} values in au, compared to gas-phase MW data.

Comp.	HF/QZVPP	MP2/QZVPP	CCSD/ QZVPP/6-31G*	CCSD/ QZVPP/6-31G**	CCSD/QZVPP/ 6-311G	CCSD/QZVPP/ TZVPP	CCSD/QZVPP	T1 Diagnostic CCSD/QZVPP/ 6-31G**
1	-0.714		-0.819	-0.819				0.014
2	-0.240	-1.462	-0.307	-0.305	-0.344			0.034
3	0.051		-0.028	-0.028	0.034	-0.164	-0.157	0.102
4	0.482	0.545	0.475	0.489	0.473			0.043
5	-0.889	-0.995	-0.779	-0.779	-0.802			0.043
6	-2.259	0.081	-1.312	-1.313	-1.284	-1.272		0.053
7	-0.787	-1.850	-0.423	-0.423	-0.411	-0.400		0.053
8	-0.114	-0.590	-0.166	-0.167	-0.184			0.027
MAE	0.3223	0.7029	0.1200	0.1184	0.1117			
ME	-0.1371	-0.2821	0.0363	0.0383	0.0385			
MaxE	1.0780	-1.4935	0.2243	0.2231	0.2503			
Slope	1.4410	0.3617	0.9990	1.0066	0.9971			

TPSS/def2-QZVPP geometries of metal complexes **1**-**8** in Cartesian coordinates (Å):

1:

Ti	-0.000817	0.000000	-0.401922
C	1.208656	0.000000	1.597687
C	0.372474	1.150679	1.596878
C	-0.980457	0.711083	1.595897
C	-0.980457	-0.711083	1.595897
C	0.372474	-1.150679	1.596878
H	2.289514	0.000000	1.582298
H	0.706583	2.178625	1.578418
H	-1.854985	1.346418	1.579197
H	-1.854985	-1.346418	1.579197
H	0.706583	-2.178625	1.578418
C	1.641763	0.000000	-1.886161
C	1.022253	-1.285731	-1.887224
C	1.022253	1.285731	-1.887224
C	-0.368401	-1.603021	-1.886486
C	-0.368401	1.603021	-1.886486
C	-1.484009	-0.713606	-1.881727
C	-1.484009	0.713606	-1.881727
H	2.717739	0.000000	-1.752912
H	1.692931	-2.126691	-1.750553
H	1.692931	2.126691	-1.750553
H	-0.607416	-2.651466	-1.747271
H	-0.607416	2.651466	-1.747271
H	-2.452795	-1.180469	-1.743556
H	-2.452795	1.180469	-1.743556

2:

Cr	-0.079081	-0.000003	-0.000171
C	1.615357	-0.060553	1.410823
C	1.626901	-1.254408	0.663146
C	1.614997	-1.191474	-0.757671
C	1.626744	0.053041	-1.417885
C	1.615631	1.251982	-0.653064
C	1.626733	1.201333	0.754760
H	1.568510	-0.102950	2.492270
H	1.587798	-2.212255	1.166046
H	1.568132	-2.106807	-1.335135
H	1.587141	0.096376	-2.498843
H	1.568860	2.209776	-1.156978
H	1.587107	2.115724	1.332882
C	-1.175786	0.376802	1.446904
C	-1.175774	1.064975	-1.049549
C	-1.175683	-1.441695	-0.397464
O	-1.851110	0.613419	2.361165
O	-1.851211	1.738652	-1.711294
O	-1.850696	-2.351938	-0.649940

3:

Mn	0.000000	0.000000	-0.056865
F	0.000000	0.000000	1.659582
O	1.492117	0.000000	-0.564123
O	-0.746059	-1.292212	-0.564123
O	-0.746059	1.292212	-0.564123

4:

Mn	0.000000	0.000000	0.158106
C	0.000000	0.000000	-1.692819
C	0.000000	1.837768	0.378283
C	-1.837768	0.000000	0.378283
C	1.837768	0.000000	0.378283
C	0.000000	-1.837768	0.378283
O	0.000000	0.000000	-2.843221
O	0.000000	2.969319	0.567659
O	-2.969319	0.000000	0.567659
O	2.969319	0.000000	0.567659
O	0.000000	-2.969319	0.567659
H	0.000000	0.000000	1.734176

5:

Mn	-0.050242	0.000234	0.000566
C	1.736452	0.821357	-0.868182
C	1.725917	1.087338	0.539993
C	1.716394	-0.163910	1.215886
C	1.717121	-1.205145	0.241447
C	1.731632	-0.586608	-1.048352
H	1.741159	1.561706	-1.654623
H	1.724482	2.062104	1.004710
H	1.696157	-0.301652	2.287429
H	1.711099	-2.266352	0.440590
H	1.726803	-1.102386	-1.997631
C	-1.041558	-1.087714	-1.030797
C	-1.071769	-0.338018	1.440784
C	-1.026012	1.443070	-0.441445
O	-1.652118	-1.803678	-1.706552
O	-1.705648	-0.560895	2.384340
O	-1.624395	2.391820	-0.731283

6:

Co	-0.173303	-0.067106	0.000000
H	-1.558680	-0.603497	0.000000
C	-1.077658	1.485642	0.000000
C	-0.112016	-0.996370	-1.537048
C	-0.112016	-0.996370	1.537048
C	1.508285	0.586815	0.000000
O	-1.701826	2.449079	0.000000
O	-0.123709	-1.604594	-2.510531
O	-0.123709	-1.604594	2.510531
O	2.576289	1.002348	0.000000

7:

Co	0.000000	0.000000	0.126774
N	0.000000	0.000000	1.785251
C	-0.000357	1.631907	-0.664545
C	1.413452	-0.815645	-0.664545
C	-1.413095	-0.816263	-0.664545
O	0.000000	0.000000	2.945542
O	0.000533	2.678490	-1.135818
O	2.319374	-1.339707	-1.135818
O	-2.319907	-1.338784	-1.135818

8:

V	0.002534	0.039193	0.000000
C	-0.980765	2.114633	0.000000
C	-0.155685	2.001251	1.149474
C	1.187133	1.818509	0.713044
C	1.187133	1.818509	-0.713044
C	-0.155685	2.001251	-1.149474
H	-2.051785	2.258781	0.000000
H	-0.489459	2.051361	2.175930
H	2.053472	1.715673	1.350139
H	2.053472	1.715673	-1.350139
H	-0.489459	2.051361	-2.175930
C	-1.788170	-0.728666	0.000000
C	-0.100230	-0.909079	-1.696346
C	-0.100230	-0.909079	1.696346
C	1.578331	-1.099246	0.000000
O	-2.854669	-1.176610	0.000000
O	-0.156024	-1.461364	-2.711388
O	-0.156024	-1.461364	2.711388
O	2.526012	-1.763256	0.000000