Supporting Information

Comparative study of electronic-structure methods for platinum-containing molecules: bond lengths and bond dissociation energies

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As mentioned in the publication we used the convention to specify the pure functional by combining the exchange functional component with the one for the correlation functional; hence, TPSSPBE denotes using the (meta GGA) TPSS exchange functional and the (pure GGA) PBE correlation functional. Please note furthermore that the names of functionals refer to the associated keyword in Gaussian16 [S1].

[S1] Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., et al. Gaussian 16 Rev. B.01. Wallingford, CT, 2016.

Table 1: Mean Average Deviation (MAD) and Standard Deviation of tested GGA density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
0HSE1PBE	0.57	0.61
B97D3	1.124	1.518
B97D	1.091	1.387
BLYP	2.806	2.686
BP86	1.482	1.971
BPBE	1.467	1.991
BPW91	1.134	1.534
BV5LYP	2.806	2.686
BVP86	1.082	1.492
G96LYP	2.258	2.253
G96P86	1.263	1.875
G96PBE	1.291	1.894
G96PW91	1.327	1.923
G96V5LYP	2.258	2.253
G96VP86	1.26	1.876
HCTH147	1.292	1.64
HCTH407	1.293	1.582
HCTH93	1.324	1.667
HCTH	1.293	1.582
mPWLYP	2.528	2.592
mPWP86	1.072	1.487

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
mPWPBE	1.427	1.976
mPWPW91	1.497	2.009
mPWV5LYP	2.528	2.592
mPWVP86	1.411	1.958
OLYP	1.546	2.09
OP86	1.675	1.831
OPBE	1.758	1.865
OPW91	1.725	1.883
OV5LYP	1.546	2.09
OVP86	1.711	1.83
PBEhLYP	2.873	2.625
PBEhP86	1.182	1.537
PBEhPBE	1.581	2.065
PBEhPW91	1.675	2.1
PBEhV5LYP	2.827	2.647
PBEhVP86	1.134	1.541
PBELYP	1.854	1.335
PBEP86	1.08	1.532
PBEPBE	1.432	1.992
PBEV5LYP	1.924	1.383
PBEVP86	0.864	1.356
PW91LYP	1.94	1.517
PW91P86	1.051	1.501
PW91PBE	1.374	1.949
PW91PW91	1.431	1.978
PW91V5LYP	1.94	1.517
PW91VP86	1.194	1.876
VSXC	1.042	1.126
wPBEhLYP	2.873	2.625
wPBEhP86	1.181	1.536
wPBEhPBE	1.581	2.065
wPBEhPW91	1.675	2.1
wPBEhV5LYP	2.884	2.632
wPBEhVP86	1.134	1.541

Table 2: Mean Average Deviation (MAD) and Standard Deviation of tested meta GGA density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
BRxB95	1.068	1.268
BRxBRC	2.063	1.362
BRxKCIS	1.415	1.424
BRxPKZB	1.097	1.271
BRxTPSS	1.058	1.268
M06L	1.178	1.29
PKZBB95	1.099	1.583
PKZBBRC	2.123	2.047
PKZBKCIS	1.226	1.644
PKZBPKZB	0.846	1.303
PKZBTPSS	0.891	1.32
tHCTH	1.259	1.706
TPSSB95	1.004	1.297
TPSSBRC	1.661	1.113
TPSSKCIS	1.191	1.37
TPSSPKZB	1.277	1.862
TPSSTPSS	0.802	1.135

Table 3: Mean Average Deviation (MAD) and Standard Deviation of tested mixed GGA/meta GGA density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
BB95	1.517	2.02
BKCIS	1.798	2.173
BPKZB	1.132	1.551
BPL	3.332	2.727
BRxLYP	2.465	1.133
BRxP86	1.046	1.23
BRxPBE	1.01	1.258
BRxPL	3.178	1.731
BRxPW91	1.097	1.265
BRxV5LYP	2.465	1.133
BRxVP86	1.002	1.232
BRxVWN5	3.105	1.75
BRxVWN	2.888	1.719
BTPSS	1.535	2.035
BVWN5	3.274	2.738
BVWN	3.104	2.708
G96B95	1.123	1.557
G96KCIS	1.545	2.057
G96PKZB	1.343	1.938
G96PL	2.904	2.601
G96TPSS	1.346	1.934
G96VWN5	2.839	2.598
G96VWN	2.674	2.57

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
mPWB95	1.486	2.004
mPWBRC	2.336	2.208
mPWPKZB	1.495	2.023
mPWPL	3.267	2.705
mPWTPSS	1.147	1.575
mPWVWN	3.036	2.682
OB95	2.137	1.925
OBRC	1.433	2.003
OKCIS	1.767	2.021
OPKZB	1.75	1.896
OPL	1.961	2.407
OTPSS	1.766	1.899
OVWN5	1.933	2.408
OVWN	1.874	2.392
PBEB95	1.541	2.01
PBEBRC	2.329	2.217
PBEhBRC	2.735	2.499
PBEhPKZB	1.192	1.611
PBEhTPSS	1.199	1.627
PBEhVWN	3.359	2.789
PBEPKZB	1.133	1.601
PBEPL	3.514	3.12
PBEPW91	1.491	2.022
PBETPSS	1.155	1.614
PBEVWN5	3.207	2.72
PBEVWN	3.036	2.69
PKZBLYP	1.647	1.117
PKZBP86	0.869	1.282
PKZBPBE	0.897	1.327
PKZBPL	2.327	1.336
PKZBPW91	0.862	1.298
PKZBV5LYP	1.647	1.117
PKZBVP86	0.87	1.289
PKZBVWN5	2.285	1.356
PKZBVWN	2.117	1.349
PW91B95	1.425	1.979
PW91BRC	2.211	2.171
PW91PKZB	1.43	1.993
PW91PL	3.143	2.666
PW91TPSS	1.133	1.575
PW91VWN5	3.076	2.66
PW91VWN	2.909	2.635
SB95	4.667	2.589
SLYP	3.164	2.2
SP86	4.493	2.612
SPBE	5.023	2.682
SPKZB	4.916	2.635
SPL	2.784	1.988

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
SPW91	4.895	2.632
STPSS	4.632	2.539
SV5LYP	3.164	2.2
SVWN5	2.863	1.992
SVWN	3.047	1.996
TPSSLYP	1.943	1.061
TPSSP86	0.848	1.115
TPSSPBE	0.792	1.14
TPSSPL	2.697	1.317
TPSSPW91	0.802	1.114
TPSSV5LYP	1.943	1.061
TPSSVP86	0.817	1.122
TPSSVWN5	2.627	1.334
TPSSVWN	2.409	1.316
wPBEhB95	1.305	1.646
wPBEhBRC	2.735	2.499
wPBEhPKZB	1.192	1.611
wPBEhTPSS	1.199	1.627
wPBEhVWN5	3.535	2.827
wPBEhVWN	3.359	2.789
XAB95	6.392	2.694
XALYP	4.687	2.176
XAP86	5.996	2.564
XAPBE	6.13	2.592
XAPKZB	6.026	2.559
XAPL	3.47	1.639
XAPW91	6.017	2.548
XATPSS	6.06	2.583
XAV5LYP	4.688	2.178
XAVP86	6.077	2.571
XAVWN5	3.555	1.641
XAVWN	4.302	1.947

Table 4: Mean Average Deviation (MAD) and Standard Deviation of tested hybrid density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
B1B95	0.9719	0.7666588
B1LYP	1.2181	1.024028
B3LYP	0.8841	0.923152
B3P86	1.0789	1.2209115
B3PW91	0.6539	0.7772215
B971	0.7651	0.8512845
B972	0.7879	0.7771917
B98	0.7461	0.8343856
mPW1LYP	1.1701	1.0085215
mPW1PBE	0.9569	0.7423722
mPW1PW91	0.8149	0.7470851
mPW3PBE	0.9769	1.2295066
O3LYP	0.6459	0.5994592
PBE1PBE	0.7259	0.6050316
SOGGA11X	3.4401	4.4861066
X3LYP	0.9091	0.8567147

Table 5: Mean Average Deviation (MAD) and Standard Deviation of tested meta hybrid density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
BMK	1.6911	1.8463507
M052X	1.9391	1.8726551
M05	2.0981	1.8992456
M062X	2.1461	2.4864378
M06HF	3.2191	2.7850306
M06	1.6361	1.591515
tHCTHhyb	0.4469	0.4728527
TPSSh	0.3039	0.3748868

Table 6: Mean Average Deviation (MAD) and Standard Deviation of tested range-separated hybrid density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
0HSE1PBE	0.5669	0.6104763
0HSE2PBE	0.5949	0.6125377
CAM-B3LYP	0.9651	1.1150066
HISSbPBE	1.1781	1.0763907
HSEH1PBE	0.5689	0.6074999
LC-wPBE	1.6111	1.7059175
M11	1.8211	1.5843312
MN12SX	0.5879	0.773077
N12SX	1.0639	1.1100292
wB97xD	1.1431	1.2872826

Table 7: Mean Average Deviation (MAD) and Standard Deviation of tested double hybrid density functionals for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
B2PLYP	1.0919	1.5
DSDPBEP86	2.5479	2.49
mPW2PLYP	1.0369	1.48
PBE0DH	1.3129	0.9
PBEQIDH	2.5979	2.11

Table 8: Mean Average Deviation (MAD) and Standard Deviation of tested ab-initio methods for bond length testset

	Bond length	
Functional	MAD (pm)	Standard Deviation (pm)
CCD	2.296	1.788
CCSD	0.978	0.815
CCSD(T)	0.618	0.563
HF	4.365	4.14
MP2	4.831	1.318
MP3	2.157	2.149
MP4	2.649	1.959

Table 9: Mean Average Deviation (MAD) and Standard Deviation of tested GGA density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
B97D3	0.703968	0.546386
B97D	0.662098	0.538224
BLYP	0.755898	0.427177
BP86	0.986399	0.454878
BPBE	0.865481	0.470062
BPW91	0.84373	0.466731
BV5LYP	0.755898	0.427177
BVP86	0.919256	0.472759
HCTH147	0.694784	0.545198
HCTH407	0.577066	0.57685
HCTH93	0.601228	0.549535
HCTH	0.577066	0.57685
HFB	0.600947	0.59808
mPWLYP	0.820313	0.426471
mPWP86	1.057295	0.451343
mPWPBE	0.936845	0.466853
mPWPW91	0.915006	0.46354
mPWV5LYP	0.820356	0.426459
mPWVP86	0.990617	0.469529
OLYP	0.608663	0.514639
OP86	0.854553	0.546738
OPBE	0.733456	0.571323
OPW91	0.710295	0.567745
OV5LYP	0.608663	0.514639
OVP86	0.788065	0.572702
PBELYP	0.889354	0.429435
PBEP86	1.13126	0.452801
PBEPBE	1.011054	0.466522
PBEPW91	0.9894	0.463283
PBEV5LYP	0.889354	0.429435
PBEVP86	1.065013	0.469162
VSXC	0.564211	0.527009

Table 10: Mean Average Deviation (MAD) and Standard Deviation of tested meta GGA density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
M06L	0.410526	0.500138
M11L	0.663866	0.379552
PKZBKCIS	0.727157	0.508373
PKZBPKZB	0.762382	0.501183
PKZBTPSS	0.692536	0.524282
tHCTH	0.63201	0.586353
TPSSKCIS	0.722127	0.441069
TPSSPKZB	0.755052	0.434907
TPSSTPSS	0.684819	0.457859

Table 11: Mean Average Deviation (MAD) and Standard Deviation of tested mixed GGA/meta GGA density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
BKCIS	0.872246	0.460004
BPKZB	0.90496	0.452772
BTPSS	0.835612	0.472364
BVWN5	0.427346	0.411233
BVWN	0.512808	0.395649
HFS	1.304806	0.63288
mPWPKZB	0.975976	0.450333
mPWTPSS	0.906588	0.469117
mPWVWN5	0.498338	0.409069
mPWVWN	0.583976	0.394143
OKCIS	0.738367	0.554557
OPKZB	0.773002	0.547074
OTPSS	0.702554	0.576926
OVWN5	0.391535	0.501818
OVWN	0.390539	0.4783
PBEPKZB	1.049896	0.451707
PBETPSS	0.980548	0.468423
PBEVWN5	0.569203	0.411153
PBEVWN	0.655399	0.397708
PKZBLYP	0.605646	0.473122
PKZBP86	0.843859	0.502875
PKZBPBE	0.723032	0.521682
PKZBPW91	0.700478	0.518092
PKZBV5LYP	0.605565	0.473114
PKZBVP86	0.777137	0.524227
PKZBVWN5	0.338335	0.456785
PKZBVWN	0.376063	0.437701
TPSSLYP	0.608096	0.408781
TPSSP86	0.835306	0.437514
TPSSPBE	0.714221	0.455794
TPSSPW91	0.69254	0.452222
TPSSV5LYP	0.608099	0.408783
TPSSVP86	0.768362	0.457797
TPSSVWN5	0.302074	0.394337
TPSSVWN	0.364154	0.376987

Table 12: Mean Average Deviation (MAD) and Standard Deviation of tested hybrid density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
B1B95	0.4299	0.5149
B1LYP	0.4633	0.5011
B3LYP	0.3577	0.4788
B3P86	0.3971	0.4795
B3PW91	0.4052	0.5058
B971	0.3213	0.4456
B972	0.3709	0.5037
B98	0.3241	0.4532
mPW1LYP	0.4359	0.4917
mPW1PBE	0.4035	0.5437
mPW1PW91	0.4054	0.5396
mPW3PBE	0.4206	0.5075
O3LYP	0.4171	0.5329
PBE1PBE	0.4282	0.5377
PBEh1PBE	0.401	0.5339
SOGGA11X	0.6442	0.5268
X3LYP	0.3931	0.519

Table 13: Mean Average Deviation (MAD) and Standard Deviation of tested meta hybrid density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
BMK	1.0197	1.565607
M052X	0.730668	0.563026
M05	0.460329	0.579404
M062X	0.848312	0.594214
M06HF	0.926548	1.00847
M06	0.499159	0.601718
tHCTHhyb	0.507466	0.527343
TPSSh	0.392694	0.492535

Table 14: Mean Average Deviation (MAD) and Standard Deviation of tested range-separated hybrid density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
CAM-B3LYP	0.496217	0.570589
HISSbPBE	0.655926	0.634333
HSEH1PBE	0.531706	0.685522
LC-wPBE	0.627912	0.797689
M11	0.92166	1.327629
MN12SX	0.345924	0.4774
N12SX	0.435271	0.56283
OHSE1PBE	0.480187	0.648549
OHSE2PBE	0.462328	0.646195
wB97xD	0.581017	0.806408

Table 15: Mean Average Deviation (MAD) and Standard Deviation of tested double hybrid density functionals for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
B2PLYP*	0.3149	0.3800
B2PLYP	0.44056	0.545678
DSDPBEP86	0.945422	0.985452
mPW2PLYP	0.380712	0.451081
PBE0DH	0.406022	0.455742
PBEQIDH	0.75581	0.885299

Table 16: Mean Average Deviation (MAD) and Standard Deviation of tested ab-initio methods for bond dissociation energy (BDE) testset

	Bond length	
Functional	MAD (eV)	Standard Deviation (eV)
HF	5.45633	2.76793
MP2	1.237577	1.476308
CCD	1.150323	0.659775
CCSD	0.752792	0.517862
CCSD(T)	0.384433	0.42405
DLPNO-CCSD(T)	0.415711	0.430159

Table 17: Determined Bond length for GGA density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
B97D3	1.736	1.686	1.679	1.901	2.153	2.055	2.078	1.521	1.866	1.759
B97D	1.736	1.686	1.679	1.901	2.153	2.055	2.078	1.521	1.872	1.763
BLYP	1.749	1.697	1.688	1.918	2.244	2.076	2.091	1.535	1.885	1.773
BP86	1.733	1.685	1.680	1.897	2.201	2.054	2.078	1.526	1.865	1.759
BPBE	1.732	1.684	1.679	1.898	2.198	2.052	2.077	1.524	1.863	1.757
BPW91	1.734	1.685	1.679	1.900	2.145	2.054	2.078	1.525	1.865	1.759
BV5LYP	1.749	1.697	1.688	1.918	2.244	2.076	2.091	1.535	1.885	1.773
BVP86	1.732	1.684	1.679	1.897	2.143	2.053	2.077	1.525	1.864	1.759
G96LYP	1.744	1.694	1.685	1.910	2.223	2.069	2.085	1.531	1.880	1.769
G96P86	1.728	1.682	1.677	1.890	2.193	2.048	2.073	1.523	1.861	1.756
G96PBE	1.728	1.681	1.676	1.890	2.191	2.046	2.072	1.520	1.858	1.754
G96PW91	1.729	1.682	1.677	1.892	2.194	2.048	2.073	1.521	1.860	1.755
G96V5LYP	1.744	1.694	1.685	1.910	2.223	2.069	2.085	1.531	1.880	1.769
G96VP86	1.728	1.681	1.676	1.889	2.192	2.047	2.072	1.522	1.859	1.755
HCTH147	1.729	1.678	1.672	1.896	2.139	2.045	2.072	1.515	1.856	1.751
HCTH407	1.727	1.675	1.669	1.883	2.136	2.040	2.072	1.513	1.851	1.747
HCTH93	1.728	1.676	1.671	1.896	2.139	2.045	2.071	1.513	1.855	1.750
HCTH	1.727	1.675	1.669	1.883	2.136	2.040	2.072	1.513	1.851	1.747
mPWLYP	1.748	1.697	1.687	1.895	2.243	2.075	2.090	1.535	1.884	1.772
mPWP86	1.732	1.684	1.679	1.896	2.143	2.053	2.077	1.526	1.864	1.759
mPWPBE	1.731	1.683	1.678	1.897	2.197	2.051	2.076	1.524	1.862	1.757
mPWPW91	1.733	1.684	1.678	1.899	2.200	2.053	2.078	1.525	1.864	1.758
mPWV5LYP	1.748	1.697	1.687	1.895	2.243	2.075	2.090	1.535	1.884	1.772
mPWVP86	1.732	1.684	1.678	1.896	2.198	2.052	2.076	1.525	1.863	1.758
OLYP	1.730	1.680	1.675	1.898	2.192	2.047	2.073	1.514	1.856	1.752
OP86	1.714	1.668	1.667	1.877	2.163	2.026	2.062	1.506	1.838	1.739
OPBE	1.714	1.668	1.666	1.877	2.160	2.024	2.061	1.504	1.836	1.737
OPW91	1.715	1.669	1.667	1.879	2.163	2.026	2.062	1.504	1.838	1.739
OV5LYP	1.730	1.680	1.675	1.898	2.192	2.047	2.073	1.514	1.856	1.752
OVP86	1.714	1.668	1.666	1.876	2.162	2.025	2.061	1.505	1.837	1.738
PBEhLYP	1.751	1.698	1.688	1.902	2.247	2.079	2.095	1.544	1.888	1.775
PBEhP86	1.735	1.685	1.680	1.903	2.149	2.057	2.082	1.530	1.868	1.761
PBEhPBE	1.735	1.684	1.679	1.903	2.202	2.055	2.081	1.528	1.865	1.759
PBEhPW91	1.736	1.685	1.679	1.905	2.205	2.057	2.082	1.529	1.867	1.760
PBEhV5LYP	1.751	1.698	1.688	1.902	2.247	2.079	2.095	1.540	1.888	1.775
PBEhVP86	1.735	1.685	1.679	1.902	2.148	2.056	2.081	1.529	1.867	1.761
PBELYP	1.748	1.696	1.687	1.897	2.174	2.074	2.091	1.536	1.883	1.771
PBEP86	1.732	1.683	1.678	1.897	2.143	2.053	2.078	1.527	1.863	1.758
PBEPBE	1.731	1.682	1.677	1.898	2.196	2.051	2.077	1.525	1.861	1.756
PBEV5LYP	1.748	1.696	1.687	1.897	2.181	2.074	2.091	1.536	1.883	1.771
PBEVP86	1.731	1.683	1.678	1.874	2.141	2.052	2.077	1.526	1.862	1.757
PW91LYP	1.746	1.695	1.686	1.915	2.172	2.073	2.089	1.535	1.882	1.771

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
PW91P86	1.731	1.683	1.678	1.895	2.140	2.052	2.076	1.526	1.862	1.757
PW91PBE	1.730	1.682	1.677	1.895	2.194	2.049	2.075	1.524	1.860	1.755
PW91PW91	1.732	1.683	1.677	1.897	2.197	2.051	2.076	1.524	1.862	1.756
PW91V5LYP	1.746	1.695	1.686	1.915	2.172	2.073	2.089	1.535	1.882	1.771
PW91VP86	1.730	1.682	1.677	1.871	2.195	2.050	2.075	1.525	1.861	1.756
VSXC	1.739	1.685	1.678	1.892	2.169	2.059	2.072	1.526	1.879	1.764
wPBEhLYP	1.751	1.698	1.688	1.902	2.247	2.079	2.095	1.544	1.888	1.775
wPBEhP86	1.735	1.685	1.680	1.903	2.149	2.057	2.082	1.530	1.868	1.761
wPBEhPBE	1.735	1.684	1.679	1.903	2.202	2.055	2.081	1.528	1.865	1.759
wPBEhPW91	1.736	1.685	1.679	1.905	2.205	2.057	2.082	1.529	1.867	1.760
wPBEhV5LYP	1.751	1.698	1.688	1.902	2.248	2.079	2.095	1.545	1.888	1.775
wPBEhVP86	1.735	1.685	1.679	1.902	2.148	2.056	2.081	1.529	1.867	1.761

Table 18: Determined Bond length for meta GGA density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
BRxB95	1.739	1.685	1.677	1.886	2.157	2.060	2.085	1.535	1.874	1.760
BRxBRC	1.750	1.696	1.687	1.902	2.181	2.077	2.096	1.539	1.889	1.772
BRxKCIS	1.741	1.687	1.679	1.896	2.166	2.065	2.093	1.534	1.877	1.763
BRxPKZB	1.737	1.685	1.678	1.888	2.161	2.061	2.087	1.534	1.876	1.760
BRxTPSS	1.737	1.685	1.678	1.886	2.159	2.060	2.087	1.533	1.875	1.760
M06L	1.738	1.682	1.672	1.890	2.163	2.060	2.086	1.531	1.876	1.765
PKZBB95	1.731	1.683	1.679	1.898	2.134	2.045	2.074	1.527	1.861	1.755
PKZBBRC	1.743	1.694	1.689	1.910	2.212	2.062	2.085	1.531	1.876	1.767
PKZBKCIS	1.733	1.684	1.682	1.904	2.143	2.050	2.082	1.525	1.865	1.758
PKZBPKZB	1.729	1.683	1.681	1.874	2.138	2.046	2.076	1.526	1.863	1.756
PKZBTPSS	1.729	1.683	1.680	1.872	2.136	2.046	2.076	1.525	1.862	1.755
tHCTH	1.728	1.678	1.673	1.886	2.132	2.040	2.067	1.513	1.847	1.749
TPSSB95	1.736	1.687	1.679	1.895	2.146	2.052	2.073	1.532	1.869	1.761
TPSSBRC	1.748	1.699	1.689	1.887	2.170	2.069	2.085	1.536	1.884	1.773
TPSSKCIS	1.738	1.689	1.682	1.901	2.155	2.057	2.082	1.530	1.872	1.763
TPSSPKZB	1.734	1.687	1.681	1.872	2.204	2.053	2.076	1.531	1.871	1.761
TPSSTPSS	1.734	1.687	1.680	1.871	2.147	2.052	2.076	1.530	1.870	1.761

Table 19: Determined Bond length for mixed GGA/meta GGA density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
BB95	1.736	1.685	1.678	1.901	2.199	2.053	2.076	1.526	1.863	1.757
BKCIS	1.738	1.686	1.680	1.907	2.205	2.058	2.084	1.525	1.866	1.760
BPKZB	1.733	1.684	1.679	1.900	2.145	2.054	2.079	1.525	1.865	1.758
BPL	1.758	1.704	1.693	1.932	2.249	2.087	2.096	1.535	1.896	1.781
BRxLYP	1.752	1.698	1.687	1.904	2.191	2.083	2.099	1.541	1.920	1.775
BRxP86	1.736	1.685	1.679	1.883	2.159	2.061	2.087	1.534	1.876	1.761
BRxPBE	1.736	1.684	1.677	1.885	2.157	2.059	2.086	1.533	1.874	1.759
BRxPL	1.761	1.704	1.691	1.922	2.212	2.093	2.105	1.543	1.907	1.783
BRxPW91	1.737	1.685	1.678	1.887	2.161	2.061	2.087	1.533	1.876	1.761
BRxV5LYP	1.752	1.698	1.687	1.904	2.191	2.083	2.099	1.541	1.920	1.775
BRxVP86	1.736	1.685	1.678	1.883	2.159	2.060	2.086	1.533	1.875	1.761
BRxVWN5	1.760	1.703	1.691	1.923	2.211	2.092	2.104	1.542	1.906	1.781
BRxVWN	1.759	1.702	1.689	1.921	2.208	2.090	2.101	1.540	1.903	1.779
BTPSS	1.733	1.684	1.679	1.900	2.200	2.053	2.078	1.525	1.864	1.758
BVWN5	1.757	1.703	1.692	1.932	2.248	2.086	2.095	1.534	1.894	1.780
BVWN	1.756	1.702	1.690	1.930	2.245	2.083	2.092	1.532	1.892	1.778
G96B95	1.731	1.681	1.675	1.893	2.134	2.047	2.070	1.523	1.858	1.754
G96KCIS	1.733	1.683	1.678	1.900	2.198	2.052	2.079	1.521	1.862	1.757
G96PKZB	1.729	1.681	1.677	1.893	2.194	2.048	2.073	1.522	1.860	1.755
G96PL	1.753	1.700	1.690	1.924	2.241	2.080	2.090	1.531	1.890	1.776
G96TPSS	1.729	1.681	1.676	1.893	2.193	2.047	2.073	1.521	1.859	1.754
G96VWN5	1.752	1.699	1.689	1.924	2.240	2.079	2.089	1.530	1.889	1.775
G96VWN	1.751	1.698	1.687	1.922	2.237	2.077	2.086	1.528	1.886	1.773
mPWB95	1.735	1.684	1.677	1.900	2.198	2.052	2.075	1.526	1.862	1.756
mPWBRC	1.747	1.696	1.687	1.912	2.218	2.070	2.087	1.531	1.877	1.769
mPWPKZB	1.733	1.684	1.678	1.899	2.200	2.053	2.078	1.525	1.864	1.757
mPWPL	1.757	1.703	1.692	1.931	2.247	2.086	2.095	1.535	1.894	1.780
mPWTPSS	1.733	1.684	1.678	1.899	2.141	2.052	2.078	1.524	1.863	1.757
mPWVWN	1.755	1.701	1.690	1.928	2.243	2.082	2.092	1.532	1.891	1.777
OB95	1.717	1.668	1.665	1.880	2.108	2.025	2.060	1.506	1.835	1.737
OBRC	1.729	1.679	1.675	1.892	2.181	2.041	2.071	1.510	1.850	1.749
OKCIS	1.719	1.670	1.668	1.887	2.167	2.030	2.068	1.504	1.839	1.740
OPKZB	1.715	1.668	1.667	1.880	2.163	2.026	2.063	1.505	1.837	1.738
OPL	1.739	1.686	1.679	1.913	2.210	2.057	2.079	1.514	1.866	1.759
OTPSS	1.715	1.668	1.666	1.880	2.162	2.026	2.062	1.504	1.837	1.738
OVWN5	1.739	1.686	1.679	1.912	2.209	2.056	2.078	1.513	1.865	1.758
OVWN	1.737	1.684	1.677	1.910	2.206	2.054	2.075	1.511	1.863	1.756
PBEB95	1.734	1.683	1.677	1.901	2.197	2.051	2.076	1.534	1.861	1.756
PBEBRC	1.746	1.695	1.686	1.913	2.217	2.069	2.088	1.531	1.876	1.768
PBEhBRC	1.750	1.697	1.688	1.919	2.233	2.074	2.092	1.535	1.880	1.772
PBEhPKZB	1.736	1.685	1.679	1.906	2.150	2.057	2.083	1.530	1.867	1.760
PBEhTPSS	1.736	1.685	1.679	1.906	2.148	2.056	2.082	1.529	1.867	1.759

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
PBEhVWN	1.759	1.702	1.691	1.935	2.249	2.087	2.097	1.536	1.895	1.780
PBEPKZB	1.732	1.683	1.678	1.900	2.143	2.052	2.079	1.526	1.863	1.757
PBEPL	1.757	1.702	1.691	1.932	2.247	2.085	2.096	1.536	1.869	1.779
PBEPW91	1.733	1.683	1.678	1.900	2.199	2.052	2.078	1.525	1.863	1.757
PBETPSS	1.732	1.683	1.677	1.900	2.142	2.052	2.078	1.525	1.862	1.756
PBEVWN5	1.756	1.701	1.690	1.932	2.246	2.084	2.096	1.535	1.892	1.778
PBEVWN	1.755	1.700	1.689	1.930	2.242	2.082	2.093	1.532	1.890	1.776
PKZBLYP	1.744	1.695	1.689	1.892	2.169	2.067	2.087	1.540	1.883	1.770
PKZBP86	1.729	1.683	1.681	1.870	2.137	2.047	2.076	1.527	1.864	1.756
PKZBPBE	1.728	1.682	1.680	1.871	2.135	2.044	2.075	1.524	1.861	1.754
PKZBPL	1.753	1.701	1.694	1.910	2.189	2.078	2.093	1.536	1.894	1.777
PKZBPW91	1.729	1.683	1.681	1.873	2.138	2.046	2.076	1.525	1.863	1.756
PKZBV5LYP	1.744	1.695	1.689	1.892	2.169	2.067	2.087	1.540	1.883	1.770
PKZBVP86	1.728	1.683	1.680	1.870	2.136	2.045	2.075	1.526	1.863	1.756
PKZBVWN5	1.753	1.701	1.693	1.910	2.189	2.077	2.092	1.535	1.893	1.777
PKZBVWN	1.751	1.699	1.691	1.908	2.186	2.075	2.089	1.532	1.890	1.775
PW91B95	1.733	1.683	1.676	1.898	2.195	2.050	2.074	1.526	1.860	1.756
PW91BRC	1.745	1.694	1.686	1.910	2.216	2.068	2.085	1.530	1.875	1.767
PW91PKZB	1.731	1.682	1.677	1.897	2.197	2.051	2.076	1.525	1.862	1.756
PW91PL	1.755	1.702	1.691	1.929	2.245	2.084	2.094	1.534	1.892	1.778
PW91TPSS	1.731	1.682	1.677	1.897	2.140	2.051	2.076	1.524	1.861	1.755
PW91VWN5	1.755	1.701	1.690	1.928	2.244	2.083	2.093	1.534	1.891	1.777
PW91VWN	1.753	1.699	1.688	1.926	2.240	2.080	2.090	1.531	1.888	1.775
SB95	1.688	1.646	1.648	1.834	2.053	1.995	2.035	1.512	1.807	1.717
SLYP	1.700	1.657	1.657	1.849	2.080	2.015	2.049	1.525	1.825	1.730
SP86	1.687	1.647	1.650	1.832	2.056	1.997	2.038	1.520	1.810	1.719
SPBE	1.686	1.646	1.649	1.799	2.054	1.995	2.037	1.510	1.808	1.717
SPKZB	1.687	1.646	1.649	1.801	2.056	1.997	2.038	1.511	1.809	1.718
SPL	1.707	1.662	1.661	1.831	2.095	2.023	2.053	1.525	1.833	1.735
SPW91	1.687	1.647	1.649	1.801	2.056	1.997	2.038	1.511	1.809	1.718
STPSS	1.687	1.646	1.649	1.833	2.054	1.996	2.038	1.510	1.808	1.717
SV5LYP	1.700	1.657	1.657	1.849	2.080	2.015	2.049	1.525	1.825	1.730
SVWN5	1.706	1.662	1.660	1.830	2.093	2.022	2.053	1.524	1.832	1.734
SVWN	1.705	1.660	1.658	1.829	2.091	2.020	2.050	1.522	1.830	1.733
TPSSLYP	1.749	1.700	1.689	1.890	2.180	2.074	2.088	1.544	1.892	1.777
TPSSP86	1.733	1.688	1.681	1.869	2.149	2.053	2.076	1.532	1.872	1.763
TPSSPBE	1.733	1.687	1.680	1.870	2.146	2.051	2.075	1.530	1.869	1.761
TPSSPL	1.758	1.706	1.694	1.907	2.201	2.085	2.093	1.541	1.902	1.785
TPSSPW91	1.734	1.688	1.681	1.872	2.149	2.053	2.076	1.531	1.871	1.762
TPSSV5LYP	1.749	1.700	1.689	1.890	2.180	2.074	2.088	1.544	1.892	1.777
TPSSVP86	1.733	1.687	1.680	1.869	2.148	2.052	2.075	1.531	1.870	1.762
TPSSVWN5	1.757	1.706	1.693	1.907	2.201	2.084	2.092	1.540	1.901	1.784

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
TPSSVWN	1.756	1.704	1.692	1.906	2.197	2.082	2.089	1.538	1.899	1.782
wPBEhB95	1.738	1.685	1.678	1.906	2.147	2.056	2.080	1.538	1.866	1.759
wPBEhBRC	1.750	1.697	1.688	1.919	2.233	2.074	2.092	1.535	1.880	1.772
wPBEhPKZB	1.736	1.685	1.679	1.906	2.150	2.057	2.083	1.530	1.867	1.760
wPBEhTPSS	1.736	1.685	1.679	1.906	2.148	2.056	2.082	1.529	1.867	1.759
wPBEhVWN5	1.760	1.704	1.692	1.937	2.253	2.089	2.100	1.538	1.897	1.782
wPBEhVWN	1.759	1.702	1.691	1.935	2.249	2.087	2.097	1.536	1.895	1.780
XAB95	1.677	1.635	1.635	1.792	2.037	1.979	2.017	1.496	1.792	1.704
XALYP	1.689	1.645	1.643	1.835	2.064	1.998	2.030	1.504	1.810	1.717
XAP86	1.676	1.635	1.636	1.818	2.040	1.981	2.020	1.497	1.794	1.706
XAPBE	1.675	1.634	1.635	1.817	2.038	1.979	2.019	1.495	1.792	1.705
XAPKZB	1.676	1.635	1.636	1.820	2.040	1.981	2.020	1.496	1.794	1.705
XAPL	1.695	1.650	1.647	1.845	2.135	2.007	2.035	1.503	1.817	1.722
XAPW91	1.676	1.635	1.636	1.819	2.040	1.981	2.020	1.495	1.794	1.705
XATPSS	1.676	1.635	1.635	1.819	2.038	1.980	2.020	1.495	1.793	1.705
XAV5LYP	1.689	1.645	1.643	1.835	2.064	1.998	2.030	1.504	1.810	1.717
XAVP86	1.675	1.635	1.636	1.817	2.039	1.980	2.019	1.496	1.793	1.706
XAVWN5	1.695	1.650	1.646	1.845	2.133	2.006	2.034	1.502	1.816	1.721
XAVWN	1.694	1.648	1.644	1.843	2.075	2.003	2.032	1.500	1.814	1.720

Table 20: Determined Bond length for hybrid density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
B1B95	1.715	1.666	1.658	1.871	2.146	2.033	2.054	1.528	1.875	1.761
B1LYP	1.729	1.680	1.670	1.891	2.179	2.056	2.069	1.535	1.919	1.776
B3LYP	1.729	1.680	1.671	1.887	2.172	2.056	2.070	1.528	1.890	1.772
B3P86	1.716	1.669	1.663	1.868	2.144	2.037	2.058	1.527	1.854	1.758
B3PW91	1.719	1.671	1.665	1.872	2.148	2.040	2.062	1.529	1.874	1.760
B971	1.723	1.676	1.669	1.880	2.164	2.053	2.064	1.524	1.885	1.768
B972	1.719	1.670	1.664	1.875	2.148	2.039	2.061	1.517	1.873	1.759
B98	1.721	1.675	1.668	1.876	2.163	2.051	2.061	1.523	1.885	1.767
mPW1LYP	1.728	1.679	1.669	1.890	2.178	2.056	2.069	1.535	1.918	1.776
mPW1PBE	1.713	1.667	1.661	1.870	2.145	2.034	2.057	1.527	1.874	1.759
mPW1PW91	1.715	1.668	1.662	1.872	2.148	2.036	2.058	1.528	1.875	1.760
mPW3PBE	1.717	1.670	1.664	1.870	2.144	2.038	2.061	1.528	1.855	1.759
O3LYP	1.722	1.673	1.667	1.880	2.145	2.040	2.064	1.513	1.896	1.754
PBE1PBE	1.713	1.666	1.660	1.870	2.145	2.034	2.058	1.527	1.898	1.758
SOGGA11X	1.716	1.719	1.657	1.923	2.224	2.172	2.060	1.525	1.896	1.775
X3LYP	1.728	1.679	1.669	1.886	2.171	2.054	2.069	1.528	1.914	1.772

Table 21: Determined Bond length for meta hybrid density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
BMK	1.702	1.656	1.649	1.861	2.180	2.053	2.044	1.529	1.909	1.768
M052X	1.707	1.656	1.643	1.884	2.179	2.019	2.028	1.513	1.900	1.754
M05	1.733	1.668	1.653	1.909	2.184	2.065	2.080	1.537	1.931	1.775
M062X	1.713	1.657	1.647	1.908	2.199	2.023	2.033	1.520	1.909	1.759
M06HF	1.682	1.645	1.644	1.888	2.179	1.980	2.001	1.500	1.893	1.748
M06	1.734	1.675	1.659	1.894	2.177	2.065	2.081	1.532	1.884	1.784
tHCTHhyb	1.723	1.676	1.671	1.869	2.148	2.049	2.064	1.523	1.899	1.762
TPSSh	1.726	1.680	1.673	1.870	2.148	2.045	2.068	1.528	1.899	1.761

Table 22: Determined Bond length for range-separated hybrid density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
0HSE1PBE	1.716	1.668	1.662	1.874	2.149	2.037	2.061	1.522	1.901	1.761
0HSE2PBE	1.716	1.668	1.661	1.875	2.149	2.037	2.060	1.520	1.901	1.760
CAM-B3LYP	1.716	1.666	1.657	1.881	2.166	2.039	2.054	1.526	1.895	1.774
HISSbPBE	1.702	1.659	1.651	1.872	2.153	2.025	2.050	1.519	1.901	1.760
HSEH1PBE	1.716	1.668	1.662	1.874	2.149	2.037	2.061	1.522	1.901	1.761
LC-wPBE	1.703	1.653	1.646	1.882	2.154	2.021	2.045	1.532	1.916	1.769
M11	1.702	1.652	1.646	1.889	2.156	2.012	2.034	1.519	1.901	1.750
MN12SX	1.715	1.678	1.678	1.859	2.153	2.043	2.065	1.531	1.906	1.771
N12SX	1.713	1.671	1.666	1.867	2.146	2.038	2.058	1.522	1.857	1.758
wB97xD	1.716	1.666	1.657	1.882	2.164	2.044	2.056	1.524	1.918	1.774

Table 23: Determined Bond length for double hybrid density functionals.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
B2PLYP	1.721	1.636	1.674	1.875	2.147	2.044	2.069	1.520	1.874	1.758
DSDPBEP86	1.694	1.586	1.662	1.864	2.137	2.023	2.056	1.512	1.865	1.749
mPW2PLYP	1.718	1.634	1.671	1.876	2.151	2.042	2.065	1.520	1.878	1.760
PBE0DH	1.707	1.647	1.659	1.868	2.142	2.025	2.053	1.520	1.895	1.755
PBEQIDH	1.696	1.595	1.654	1.861	2.131	2.018	2.048	1.511	1.885	1.745

Table 24: Determined Bond length for ab-initio methods.

	PtO	PtN	PtC	PtF	PtCl	PtS	PtSi	PtH	PtCN	PtCO
Exp.	1.727	1.682	1.678	1.874	2.153	2.040	2.062	1.528	1.899	1.760
CCD	1.679	1.646	1.637	1.875	2.163	2.019	2.035	1.502	1.881	1.758
CCSD	1.716	1.670	1.657	1.873	2.156	2.029	2.048	1.508	1.902	1.758
CCSD(T)	1.717	1.683	1.672	1.870	2.144	2.036	2.062	1.508	1.894	1.757
HF	1.762	1.689	1.664	1.943	2.283	2.054	2.064	1.552	1.972	1.829
MP2	1.658	1.624	1.631	1.846	2.099	1.999	2.030	1.483	1.831	1.720
MP3	1.689	1.657	1.635	1.877	2.176	2.028	2.030	1.504	1.908	1.768
MP4	1.673	1.661	1.690	1.858	2.123	2.024	2.062	1.501	1.850	1.720

Table 25: Determined bond dissociation energies for GGA density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
B97D3	6.83	6.75	4.10	3.66	4.71	4.09	3.12	4.13	4.75	3.49
B97D	6.76	6.68	4.10	3.60	4.66	4.04	3.07	4.06	4.70	3.45
BLYP	6.66	6.74	4.39	4.04	4.75	4.24	3.04	3.99	5.11	3.90
BP86	7.00	7.11	4.60	4.28	4.96	4.48	3.37	4.35	5.37	4.18
BPBE	6.85	6.96	4.38	4.07	4.81	4.34	3.31	4.25	5.20	3.98
BPW91	6.82	6.93	4.35	4.04	4.78	4.32	3.29	4.21	5.18	3.97
BV5LYP	6.66	6.74	4.39	4.04	4.75	4.24	3.04	3.99	5.11	3.90
BVP86	6.88	7.02	4.44	4.16	4.87	4.44	3.37	4.32	5.26	4.05
HCTH147	6.81	6.76	4.08	3.62	4.70	4.12	3.12	4.10	4.77	3.50
HCTH407	6.59	6.60	3.76	3.37	4.53	4.02	3.08	4.02	4.61	3.34
HCTH93	6.66	6.66	3.92	3.51	4.56	4.03	3.03	3.99	4.66	3.40
HCTH	6.59	6.60	3.76	3.37	4.53	4.02	3.08	4.02	4.61	3.34
HFB	5.21	5.53	2.66	2.61	3.52	3.34	2.43	3.18	3.79	2.58
mPWLYP	6.74	6.82	4.47	4.13	4.83	4.33	3.11	4.07	5.20	3.99
mPWP86	7.09	7.19	4.70	4.38	5.05	4.57	3.44	4.44	5.46	4.27
mPWPBE	6.94	7.05	4.48	4.16	4.90	4.43	3.38	4.33	5.29	4.08
mPWPW91	6.91	7.02	4.45	4.14	4.88	4.41	3.35	4.30	5.27	4.06
mPWV5LYP	6.74	6.82	4.47	4.13	4.83	4.33	3.11	4.07	5.20	3.99
mPWVP86	6.97	7.11	4.54	4.25	4.97	4.53	3.43	4.40	5.35	4.14
OLYP	6.57	6.65	4.00	3.66	4.54	4.07	3.02	3.92	4.73	3.49
OP86	6.92	7.03	4.23	3.93	4.76	4.33	3.36	4.30	5.01	3.78
OPBE	6.77	6.89	4.00	3.71	4.61	4.19	3.31	4.19	4.84	3.59
OPW91	6.74	6.85	3.98	3.69	4.59	4.16	3.28	4.16	4.82	3.57
OV5LYP	6.57	6.65	4.00	3.66	4.54	4.07	3.02	3.92	4.73	3.49
OVP86	6.80	6.95	4.06	3.81	4.68	4.28	3.36	4.27	4.90	3.66
PBELYP	6.83	6.92	4.58	4.23	4.91	4.41	3.16	4.14	5.27	4.07
PBEP86	7.19	7.29	4.82	4.49	5.14	4.66	3.49	4.50	5.54	4.35
PBEPBE	7.05	7.15	4.60	4.27	5.00	4.52	3.44	4.40	5.37	4.16
PBEPW91	7.02	7.12	4.57	4.24	4.97	4.49	3.41	4.36	5.35	4.15
PBEV5LYP	6.83	6.92	4.58	4.23	4.91	4.41	3.16	4.14	5.27	4.07
PBEVP86	7.08	7.21	4.66	4.36	5.06	4.61	3.49	4.47	5.43	4.23
VSXC	6.66	6.56	3.91	3.39	4.65	4.01	2.99	3.97	4.71	3.30

Table 26: Determined bond dissociation energies for meta GGA density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
M06L	6.35	6.11	3.64	3.03	4.24	3.51	2.81	3.75	4.49	3.08
M11L	5.50	5.07	2.94	2.11	3.63	2.55	2.01	2.99	4.19	2.54
PKZBKCIS	6.73	6.85	4.18	3.89	4.58	4.15	3.11	4.07	4.92	3.72
PKZBPKZB	6.78	6.90	4.25	3.96	4.64	4.19	3.13	4.10	4.98	3.74
PKZBTPSS	6.66	6.77	4.08	3.78	4.57	4.13	3.17	4.10	4.84	3.60
tHCTH	6.71	6.67	3.93	3.47	4.61	4.04	3.15	4.13	4.62	3.32
TPSSKCIS	6.68	6.73	4.29	3.92	4.65	4.10	3.14	4.05	5.07	3.82
TPSSPKZB	6.73	6.77	4.36	3.99	4.70	4.13	3.15	4.08	5.12	3.85
TPSSTPSS	6.60	6.65	4.19	3.81	4.63	4.07	3.19	4.08	4.98	3.70

Table 27: Determined bond dissociation energies for mixed GGA/meta GGA density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
	6.89	6.99	4.42	4.09	4.82	4.34	3.24	4.20	5.23	4.05
BKCIS	6.89	6.99	4.42	4.09	4.82	4.34	3.24	4.20	5.23	4.05
BPKZB	6.94	7.03	4.49	4.15	4.87	4.38	3.26	4.23	5.29	4.07
BTPSS	6.82	6.91	4.32	3.98	4.81	4.32	3.29	4.23	5.16	3.93
BVWN5	6.28	6.32	3.97	3.59	4.35	3.79	2.68	3.59	4.76	3.55
BVWN	6.42	6.43	4.15	3.73	4.47	3.86	2.72	3.65	4.91	3.70
HFS	7.15	7.52	4.31	4.30	5.35	5.25	4.04	5.16	5.69	4.45
mPWPKZB	7.04	7.12	4.59	4.25	4.97	4.47	3.33	4.31	5.38	4.17
mPWTPSS	6.91	6.99	4.42	4.07	4.90	4.41	3.36	4.31	5.25	4.02
mPWVWN5	6.37	6.41	4.07	3.68	4.45	3.88	2.75	3.67	4.85	3.64
mPWVWN	6.51	6.52	4.25	3.82	4.57	3.95	2.79	3.73	5.00	3.79
OKCIS	6.81	6.91	4.04	3.73	4.63	4.19	3.24	4.14	4.87	3.66
OPKZB	6.87	6.95	4.11	3.80	4.68	4.23	3.25	4.17	4.93	3.68
OTPSS	6.75	6.83	3.94	3.62	4.61	4.17	3.29	4.17	4.79	3.54
OVWN5	6.18	6.23	3.57	3.20	4.13	3.61	2.65	3.50	4.37	3.13
OVWN	6.32	6.34	3.75	3.34	4.25	3.68	2.69	3.56	4.52	3.28
PBEPKZB	7.14	7.21	4.71	4.35	5.06	4.56	3.38	4.38	5.46	4.25
PBETPSS	7.02	7.09	4.53	4.18	4.99	4.50	3.42	4.38	5.33	4.11
PBEVWN5	6.47	6.51	4.18	3.79	4.53	3.97	2.80	3.73	4.93	3.73
PBEVWN	6.61	6.62	4.36	3.93	4.65	4.04	2.84	3.80	5.08	3.88
PKZBLYP	6.49	6.60	4.14	3.83	4.51	4.04	2.91	3.86	4.78	3.56
PKZBP86	6.83	6.98	4.36	4.09	4.72	4.29	3.24	4.23	5.06	3.85
PKZBPBE	6.69	6.83	4.14	3.87	4.57	4.15	3.19	4.12	4.89	3.65
PKZBPW91	6.65	6.80	4.11	3.85	4.55	4.13	3.16	4.09	4.87	3.63
PKZBV5LYP	6.49	6.60	4.14	3.83	4.51	4.04	2.91	3.86	4.78	3.56
PKZBVP86	6.72	6.89	4.20	3.96	4.63	4.25	3.24	4.19	4.94	3.72
PKZBVWN5	6.10	6.18	3.72	3.38	4.10	3.59	2.55	3.45	4.44	3.21
PKZBVWN	6.25	6.29	3.90	3.51	4.22	3.66	2.59	3.51	4.59	3.36
TPSSLYP	6.45	6.48	4.27	3.87	4.58	4.00	2.95	3.85	4.94	3.68
TPSSP86	6.78	6.85	4.47	4.12	4.78	4.23	3.27	4.20	5.20	3.95
TPSSPBE	6.63	6.70	4.25	3.90	4.63	4.09	3.21	4.09	5.03	3.75
TPSSPW91	6.60	6.67	4.23	3.87	4.61	4.07	3.18	4.06	5.01	3.74
TPSSV5LYP	6.45	6.48	4.27	3.87	4.58	4.00	2.95	3.85	4.94	3.68
TPSSVP86	6.66	6.77	4.31	3.99	4.69	4.19	3.26	4.17	5.09	3.82
TPSSVWN5	6.06	6.06	3.85	3.42	4.18	3.55	2.59	3.44	4.59	3.32
TPSSVWN	6.20	6.17	4.02	3.56	4.29	3.61	2.63	3.50	4.74	3.48

Table 28: Determined bond dissociation energies for hybrid density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
B1B95	6.06	5.97	3.37	2.87	3.97	3.33	2.75	3.25	4.24	2.61
B1LYP	5.67	5.62	3.22	2.75	3.73	3.10	2.52	2.94	3.94	2.35
B3LYP	5.97	5.93	3.53	3.07	4.02	3.39	2.67	3.23	4.28	2.77
B3P86	6.29	6.25	3.75	3.28	4.24	3.61	2.95	3.54	4.54	3.02
B3PW91	6.10	6.06	3.51	3.05	4.06	3.44	2.84	3.39	4.32	2.80
B971	6.22	6.08	3.68	3.12	4.18	3.49	2.46	3.35	4.40	2.86
B972	6.25	6.07	3.58	2.98	4.14	3.41	2.35	3.39	4.21	2.64
B98	6.12	6.00	3.56	3.02	4.10	3.43	2.43	3.30	4.31	2.76
mPW1LYP	5.73	5.68	3.29	2.82	3.80	3.17	2.57	3.00	4.01	2.42
mPW1PBE	5.96	5.91	3.33	2.86	3.90	3.27	2.81	3.25	4.11	2.52
mPW1PW91	5.92	5.87	3.30	2.83	3.87	3.24	2.79	3.22	4.09	2.50
mPW3PBE	6.19	6.15	3.60	3.14	4.14	3.53	2.92	3.48	4.40	2.88
O3LYP	6.21	6.23	3.58	3.19	4.18	3.64	2.82	3.52	4.31	2.89
PBE1PBE	6.04	5.98	3.41	2.94	3.96	3.34	2.86	3.31	4.18	2.59
PBEh1PBE	5.99	5.93	3.37	2.90	3.93	3.30	2.83	3.28	4.16	2.57
SOGGA11X	5.61	5.48	2.96	2.44	3.51	2.86	2.16	2.72	3.68	1.89
X3LYP	5.94	5.89	3.49	3.03	3.99	3.36	2.67	3.20	4.24	2.69

Table 29: Determined bond dissociation energies for meta hybrid density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
M052X	5.63	5.47	2.81	2.21	3.51	2.74	2.13	2.47	3.59	1.66
M05	6.00	5.68	3.21	2.50	3.87	3.01	2.40	3.09	3.86	2.17
M062X	5.46	5.47	2.59	2.21	3.19	2.65	1.85	2.37	3.45	1.61
M06HF	6.72	5.21	3.78	1.83	4.21	1.15	1.85	1.59	2.80	2.17
M06	6.06	5.85	3.23	2.67	3.85	3.17	2.63	3.39	4.20	2.51
tHCTHhyb	6.45	6.39	3.83	3.35	4.39	3.78	3.02	3.72	4.56	3.08
TPSSh	6.24	6.24	3.75	3.32	4.25	3.65	2.99	3.68	4.53	3.10

Table 30: Determined bond dissociation energies for range-separated hybrid density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
CAM-B3LYP	5.64	5.58	3.23	2.73	2.64	3.87	2.28	2.88	5.39	2.43
HISSbPBE	5.38	5.27	2.77	2.23	2.19	3.50	2.29	2.71	5.12	2.03
HSEH1PBE	6.01	5.95	3.39	2.92	2.65	3.94	2.85	3.31	5.46	2.60
LC-wPBE	6.95	5.30	4.55	2.45	4.11	5.36	2.19	2.58	5.47	4.00
M11	7.21	5.46	4.60	2.37	3.95	5.06	2.04	2.51	4.82	-0.31
MN12SX	6.27	5.67	3.61	2.60	3.18	4.08	2.52	3.18	5.50	2.85
N12SX	6.11	5.93	3.42	2.83	3.01	4.18	2.64	3.40	5.66	2.93
OHSE1PBE	6.01	5.95	3.39	2.92	2.65	3.94	2.85	3.31	5.38	2.60
OHSE2PBE	6.00	5.95	3.38	2.91	2.64	3.94	2.84	3.30	5.46	2.59
wB97xD	5.86	5.66	3.30	2.68	2.74	3.94	2.27	3.03	5.32	0.87

Table 31: Determined bond dissociation energies for double hybrid density functionals

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
B2PLYP	6.62	6.36	3.81	3.21	4.25	3.38	2.39	3.67	5.26	4.63
DSDPBEP86	8.06	6.36	4.82	2.84	5.32	1.91	2.43	3.75	5.57	4.98
mPW2PLYP	6.40	6.15	3.59	2.99	4.08	3.22	2.34	3.48	4.95	4.06
PBE0DH	5.97	5.79	3.15	2.59	3.73	2.98	2.34	3.13	4.18	2.71
PBEQIDH	7.80	6.04	4.61	2.53	5.30	1.80	2.36	3.41	4.73	3.72

Table 32: Determined bond dissociation energies for ab-initio methods.

	PtC	PtC^+	PtN	PtN^+	PtO	PtO^+	$PtCO^+$	$PtNO^+$	$OPtO$	$OPtO^+$
Exp.	5.95	5.46	3.84	3.35	4.3	3.26	2.28	3.13	5.54	4.06
HF	1.55	1.56	0.00	-7.45	0.06	0.58	-0.06	-7.04	-0.40	-3.17
MP2	7.75	7.10	3.27	2.49	4.45	2.99	2.95	4.89	9.69	2.56
CCD	5.40	5.01	1.85	1.10	3.02	1.90	2.19	2.44	3.98	1.77
CCSD	5.65	5.33	2.85	2.18	3.43	2.68	2.29	2.52	3.73	2.02
CCSD(T)	6.39	6.01	3.49	2.76	3.99	3.13	2.52	3.27	4.82	3.44
DLPNO-CCSD(T)	6.12	5.86	3.30	2.65	3.78	2.95	2.44	2.98	4.65	3.36

*Table 33: Initial parameters for calculations (BL-Testset)**

Molecule	Charge	Spin	Atom	x-coordinate	y-coordinate	z-coordinate
PtO	0	3	Pt	-0.62030078	-0.07518797	0.00000000
			O	-2.57030078	-0.07518797	0.00000000
PtN	0	2	Pt	-1.20300756	-0.07518797	0.00000000
			N	-3.19300756	-0.07518797	0.00000000
PtC	0	1	Pt	-1.54082525	0.41353383	-0.04034793
			C	-3.60082525	0.41353383	-0.04034793
PtF	0	2	Pt	-0.14675052	0.11530398	0.00000000
			F	-2.00533981	0.32157041	0.00000000
$PtCl$	0	2	Pt	-0.14675052	0.11530398	0.00000000
			Cl	-2.41283800	0.36679460	0.00000000
PtS	0	3	Pt	-0.54511280	0.09398496	0.00000000
			S	-2.84511280	0.09398496	0.00000000
$PtSi$	0	1	Pt	-0.24390244	-0.24390244	0.00000000
			Si	-2.70390244	-0.24390244	0.00000000
PtH	0	2	Pt	-0.14675052	0.11530398	0.00000000
			H	1.44324948	0.11530398	0.00000000
$PtCN$	0	2	Pt	-1.59249609	0.15244454	0.00000000
			C	0.37707317	0.75609755	0.00000000
			N	1.74721983	1.28863686	0.00000000
$PtCO$	0	1	Pt	-1.59249609	0.15244454	0.00000000
			C	0.37707317	0.75609755	0.00000000
			O	1.70993693	1.27414600	0.00000000

*Please note that the input geometry might be slightly changed for a small number of calculations since it was necessary because of convergence issues.

*Table 34: Initial parameters for calculations (BDE-Testset)**

Molecule	Charge	Spin	Atom	x-coordinate	y-coordinate	z-coordinate
PtC	0	1	Pt	-2.513737000000	0.024390000000	0.000000000000
			O	-0.840897000000	0.024390000000	0.000000000000
PtC^+	1	2	Pt	2.234316000000	0.672269000000	0.000000000000
			C	2.234316000000	0.672269000000	0.000000000000
PtN	0	2	Pt	-0.398992000000	-0.219512000000	0.000000000000
			N	-2.078813000000	-0.219512000000	0.000000000000
PtN^+	1	3	Pt	-0.397540000000	-0.219512000000	0.000000000000
			N	-2.080265000000	-0.219512000000	0.000000000000
PtO	0	3	Pt	-1.796481000000	-0.268293000000	0.000000000000
			O	-3.519373000000	-0.268293000000	0.000000000000
PtO^+	1	4	Pt	-1.793835000000	-0.268293000000	0.000000000000
			O	-3.522019000000	-0.268293000000	0.000000000000
$PtCO^+$	1	2	Pt	0.475803000000	0.902742000000	0.140661000000
			C	2.311672000000	1.201996000000	0.208998000000
			O	3.418394000000	1.381721000000	0.250341000000
$PtNO^+$	1	1	Pt	-2.111271000000	-0.652809000000	0.000000000000
			N	-0.485818000000	-0.038962000000	0.000000000000
			O	0.553195000000	0.370402000000	0.000000000000
$OPtO$	0	1	Pt	-2.585366000000	0.219512000000	0.009513000000
			O	-4.282170000000	0.219512000000	0.021959000000
			O	-0.888562000000	0.219512000000	0.021959000000
$OPtO^+$	1	2	Pt	-2.585366000000	0.219512000000	0.009817000000
			O	-4.272994000000	0.219512000000	0.021807000000
			O	-0.897738000000	0.219512000000	0.021807000000

*Please note that the input geometry might be slightly changed for a small number of calculations since it was necessary because of convergence issues.