

9 Supporting Information

Table V. A comparison of the optimized geometric parameters for the group 14 congeners of the formic acid molecule represented in Figure 1. Bond lengths are in angstroms and angles in degrees.

	Method/Basis	X = C	X = Si	X = Ge	X = Sn	X = Pb
r ₁	B3LYP/DZP	0.976	0.970	0.972	—	—
r ₁	BLYP/DZP	0.987	0.980	0.983	—	—
r ₁	B3LYP/DZP-ECP	—	0.970	0.971	0.969	0.971
r ₁	BLYP/DZP-ECP	—	0.981	0.981	0.980	0.982
r ₁	B3LYP/TZ2P	0.970	0.963	0.964	—	—
r ₁	BLYP/TZ2P	0.981	0.973	0.975	—	—
r ₁	B3LYP/TZ2P-ECP	—	0.962	0.963	0.961	0.962
r ₁	BLYP/TZ2P-ECP	—	0.972	0.973	0.972	0.973
r ₂	B3LYP/DZP	1.351	1.629	1.769	—	—
r ₂	BLYP/DZP	1.371	1.649	1.796	—	—
r ₂	B3LYP/DZP-ECP	—	1.646	1.750	1.910	1.995
r ₂	BLYP/DZP-ECP	—	1.664	1.773	1.934	2.024
r ₂	B3LYP/TZ2P	1.346	1.626	1.774	—	—
r ₂	BLYP/TZ2P	1.366	1.646	1.803	—	—
r ₂	B3LYP/TZ2P-ECP	—	1.643	1.751	1.916	1.998
r ₂	BLYP/TZ2P-ECP	—	1.662	1.775	1.941	2.028
r ₃	B3LYP/DZP	1.210	1.521	1.637	—	—
r ₃	BLYP/DZP	1.222	1.539	1.658	—	—
r ₃	B3LYP/DZP-ECP	—	1.527	1.622	1.783	1.833
r ₃	BLYP/DZP-ECP	—	1.544	1.641	1.803	1.853
r ₃	B3LYP/TZ2P	1.197	1.518	1.642	—	—
r ₃	BLYP/TZ2P	1.209	1.535	1.664	—	—
r ₃	B3LYP/TZ2P-ECP	—	1.532	1.626	1.789	1.837
r ₃	BLYP/TZ2P-ECP	—	1.549	1.644	1.809	1.858
r ₄	B3LYP/DZP	1.103	1.468	1.528	—	—
r ₄	BLYP/DZP	1.111	1.479	1.542	—	—
r ₄	B3LYP/DZP-ECP	—	1.450	1.522	1.693	1.713

r_4	BLYP/DZP-ECP	—	1.460	1.533	1.704	1.727
r_4	B3LYP/TZ2P	1.095	1.466	1.529	—	—
r_4	BLYP/TZ2P	1.103	1.476	1.543	—	—
r_4	B3LYP/TZ2P-ECP	—	1.460	1.528	1.701	1.722
r_4	BLYP/TZ2P-ECP	—	1.469	1.538	1.712	1.737
θ_1	B3LYP/DZP	107.3	117.8	112.2	—	—
θ_1	BLYP/DZP	106.6	116.6	110.9	—	—
θ_1	B3LYP/DZP-ECP	—	117.5	115.0	117.1	113.4
θ_1	BLYP/DZP-ECP	—	116.2	113.6	115.3	111.7
θ_1	B3LYP/TZ2P	107.6	117.2	111.9	—	—
θ_1	BLYP/TZ2P	107.0	116.2	110.6	—	—
θ_1	B3LYP/TZ2P-ECP	—	115.8	113.4	115.3	112.0
θ_1	BLYP/TZ2P-ECP	—	114.8	112.3	113.9	110.4
θ_2	B3LYP/DZP	125.2	127.9	124.4	—	—
θ_2	BLYP/DZP	125.4	128.3	124.8	—	—
θ_2	B3LYP/DZP-ECP	—	126.6	125.1	123.6	117.1
θ_2	BLYP/DZP-ECP	—	127.0	125.4	123.6	116.6
θ_2	B3LYP/TZ2P	125.2	128.0	124.2	—	—
θ_2	BLYP/TZ2P	125.4	128.5	124.6	—	—
θ_2	B3LYP/TZ2P-ECP	—	126.7	125.0	123.9	117.3
θ_2	BLYP/TZ2P-ECP	—	127.1	125.3	123.9	116.9
θ_3	B3LYP/DZP	125.4	127.5	131.9	—	—
θ_3	BLYP/DZP	125.9	127.8	132.3	—	—
θ_3	B3LYP/DZP-ECP	—	128.6	131.3	135.0	145.9
θ_3	BLYP/DZP-ECP	—	128.9	131.8	135.8	147.1
θ_3	B3LYP/TZ2P	125.2	127.1	131.9	—	—
θ_3	BLYP/TZ2P	125.6	127.3	132.2	—	—
θ_3	B3LYP/TZ2P-ECP	—	128.9	131.3	134.9	145.5
θ_3	BLYP/TZ2P-ECP	—	129.1	131.7	135.5	146.4

Table VI. A comparison of the optimized geometric parameters for the group 14 congeners of the hydroperoxycarbene molecule represented in Figure 2. Bond lengths are in angstroms and angles in degrees.

Parameter	Method/Basis	X = C	X = Si	X = Ge	X = Sn	X = Pb
r ₁	B3LYP/DZP	0.975	0.975	0.974	—	—
r ₁	BLYP/DZP	0.987	0.987	0.986	—	—
r ₁	B3LYP/DZP-ECP	—	0.975	0.974	0.973	0.973
r ₁	BLYP/DZP-ECP	—	0.987	0.986	0.985	0.985
r ₁	B3LYP/TZ2P	0.966	0.967	0.966	—	—
r ₁	BLYP/TZ2P	0.977	0.978	0.978	—	—
r ₁	B3LYP/TZ2P-ECP	—	0.967	0.966	0.965	0.964
r ₁	BLYP/TZ2P-ECP	—	0.978	0.977	0.976	0.976
r ₂	B3LYP/DZP	1.775	1.472	1.461	—	—
r ₂	BLYP/DZP	1.851	1.536	1.503	—	—
r ₂	B3LYP/DZP-ECP	—	1.472	1.462	1.460	1.459
r ₂	BLYP/DZP-ECP	—	1.536	1.506	1.497	1.491
r ₂	B3LYP/TZ2P	1.847	1.478	1.465	—	—
r ₂	BLYP/TZ2P	1.912	1.558	1.513	—	—
r ₂	B3LYP/TZ2P-ECP	—	1.477	1.467	1.465	1.463
r ₂	BLYP/TZ2P-ECP	—	1.557	1.520	1.508	1.501
r ₃	B3LYP/DZP	1.196	1.669	1.809	—	—
r ₃	BLYP/DZP	1.204	1.675	1.829	—	—
r ₃	B3LYP/DZP-ECP	—	1.687	1.801	1.966	2.048
r ₃	BLYP/DZP-ECP	—	1.688	1.816	1.985	2.072
r ₃	B3LYP/TZ2P	1.168	1.664	1.815	—	—
r ₃	BLYP/TZ2P	1.178	1.665	1.835	—	—
r ₃	B3LYP/TZ2P-ECP	—	1.681	1.798	1.966	2.048
r ₃	BLYP/TZ2P-ECP	—	1.680	1.810	1.985	2.072
r ₄	B3LYP/DZP	1.107	1.526	1.596	—	—
r ₄	BLYP/DZP	1.114	1.538	1.612	—	—
r ₄	B3LYP/DZP-ECP	—	1.515	1.601	1.770	1.820
r ₄	BLYP/DZP-ECP	—	1.525	1.612	1.782	1.833
r ₄	B3LYP/TZ2P	1.097	1.525	1.601	—	—
r ₄	BLYP/TZ2P	1.104	1.535	1.618	—	—

r_4	B3LYP/TZ2P-ECP	—	1.521	1.607	1.779	1.831
r_4	BLYP/TZ2P-ECP	—	1.529	1.618	1.790	1.844
θ_1	B3LYP/DZP	98.6	98.8	99.1	—	—
θ_1	BLYP/DZP	97.0	97.3	97.9	—	—
θ_1	B3LYP/DZP-ECP	—	98.7	98.9	99.0	99.0
θ_1	BLYP/DZP-ECP	—	97.2	97.7	97.8	98.0
θ_1	B3LYP/TZ2P	100.6	99.0	99.3	—	—
θ_1	BLYP/TZ2P	99.0	97.3	98.1	—	—
θ_1	B3LYP/TZ2P-ECP	—	99.2	99.4	99.4	99.4
θ_1	BLYP/TZ2P-ECP	—	97.5	98.0	98.2	98.3
θ_2	B3LYP/DZP	114.8	119.0	116.8	—	—
θ_2	BLYP/DZP	116.4	119.8	117.3	—	—
θ_2	B3LYP/DZP-ECP	—	117.8	117.7	117.4	116.8
θ_2	BLYP/DZP-ECP	—	118.6	118.4	117.9	117.2
θ_2	B3LYP/TZ2P	112.9	119.0	116.7	—	—
θ_2	BLYP/TZ2P	114.5	119.9	117.3	—	—
θ_2	B3LYP/TZ2P-ECP	—	117.8	117.4	116.8	116.1
θ_2	BLYP/TZ2P-ECP	—	118.6	118.0	117.2	116.4
θ_3	B3LYP/DZP	122.2	98.1	96.0	—	—
θ_3	BLYP/DZP	124.5	99.7	96.7	—	—
θ_3	B3LYP/DZP-ECP	—	97.7	96.4	95.8	96.2
θ_3	BLYP/DZP-ECP	—	99.3	97.3	96.5	96.9
θ_3	B3LYP/TZ2P	125.8	98.3	96.0	—	—
θ_3	BLYP/TZ2P	127.0	100.2	96.9	—	—
θ_3	B3LYP/TZ2P-ECP	—	97.8	96.3	96.0	96.4
θ_3	BLYP/TZ2P-ECP	—	99.8	97.3	96.8	97.2

Table VII. A comparison of the geometric parameters for the group 14 congeners of the acetic acid molecule represented in Figure 3. Bond lengths are in angstroms and angles in degrees.

Parameter	Method/Basis	X = C	X = Si	X = Ge	X = Sn	X = Pb
r ₁	B3LYP/DZP	0.975	0.969	0.971	—	—
r ₁	BLYP/DZP	0.986	0.979	0.982	—	—
r ₁	B3LYP/DZP-ECP	—	0.970	0.970	0.969	0.970
r ₁	BLYP/DZP-ECP	—	0.980	0.981	0.980	0.982
r ₁	B3LYP/TZ2P	0.968	0.962	0.964	—	—
r ₁	BLYP/TZ2P	0.979	0.972	0.974	—	—
r ₁	B3LYP/TZ2P-ECP	—	0.961	0.962	0.961	0.962
r ₁	BLYP/TZ2P-ECP	—	0.972	0.973	0.972	0.973
r ₂	B3LYP/DZP	1.362	1.637	1.776	—	—
r ₂	BLYP/DZP	1.383	1.657	1.805	—	—
r ₂	B3LYP/DZP-ECP	—	1.655	1.759	1.918	2.004
r ₂	BLYP/DZP-ECP	—	1.674	1.782	1.942	2.033
r ₂	B3LYP/TZ2P	1.358	1.634	1.782	—	—
r ₂	BLYP/TZ2P	1.380	1.655	1.813	—	—
r ₂	B3LYP/TZ2P-ECP	—	1.650	1.760	1.925	2.009
r ₂	BLYP/TZ2P-ECP	—	1.670	1.784	1.950	2.039
r ₃	B3LYP/DZP	1.215	1.524	1.641	—	—
r ₃	BLYP/DZP	1.227	1.542	1.662	—	—
r ₃	B3LYP/DZP-ECP	—	1.532	1.626	1.786	1.840
r ₃	BLYP/DZP-ECP	—	1.548	1.644	1.806	1.861
r ₃	B3LYP/TZ2P	1.203	1.521	1.647	—	—
r ₃	BLYP/TZ2P	1.215	1.539	1.669	—	—
r ₃	B3LYP/TZ2P-ECP	—	1.535	1.630	1.793	1.843
r ₃	BLYP/TZ2P-ECP	—	1.552	1.648	1.813	1.865
r ₄	B3LYP/DZP	1.511	1.854	1.945	—	—
r ₄	BLYP/DZP	1.523	1.871	1.971	—	—
r ₄	B3LYP/DZP-ECP	—	1.862	1.945	2.124	2.180
r ₄	BLYP/DZP-ECP	—	1.876	1.964	2.145	2.211
r ₄	B3LYP/TZ2P	1.503	1.851	1.946	—	—
r ₄	BLYP/TZ2P	1.514	1.868	1.973	—	—

r_4	B3LYP/TZ2P-ECP	—	1.850	1.938	2.122	2.174
r_4	BLYP/TZ2P-ECP	—	1.865	1.958	2.145	2.205
r_5	B3LYP/DZP	1.092	1.094	1.093	—	—
r_5	BLYP/DZP	1.099	1.101	1.100	—	—
r_5	B3LYP/DZP-ECP	—	1.093	1.093	1.093	1.092
r_5	BLYP/DZP-ECP	—	1.100	1.100	1.099	1.098
r_5	B3LYP/TZ2P	1.084	1.087	1.085	—	—
r_5	BLYP/TZ2P	1.091	1.093	1.091	—	—
r_5	B3LYP/TZ2P-ECP	—	1.084	1.084	1.085	1.083
r_5	BLYP/TZ2P-ECP	—	1.091	1.091	1.091	1.089
r_6	B3LYP/DZP	1.096	1.097	1.095	—	—
r_6	BLYP/DZP	1.104	1.104	1.102	—	—
r_6	B3LYP/DZP-ECP	—	1.096	1.095	1.095	1.093
r_6	BLYP/DZP-ECP	—	1.103	1.102	1.101	1.100
r_6	B3LYP/TZ2P	1.090	1.090	1.088	—	—
r_6	BLYP/TZ2P	1.096	1.096	1.094	—	—
r_6	B3LYP/TZ2P-ECP	—	1.088	1.087	1.087	1.085
r_6	BLYP/TZ2P-ECP	—	1.094	1.093	1.093	1.090
θ_1	B3LYP/DZP	106.2	116.3	111.4	—	—
θ_1	BLYP/DZP	105.4	115.1	109.9	—	—
θ_1	B3LYP/DZP-ECP	—	116.1	114.2	116.7	113.3
θ_1	BLYP/DZP-ECP	—	114.8	112.7	114.7	111.4
θ_1	B3LYP/TZ2P	106.8	115.7	111.2	—	—
θ_1	BLYP/TZ2P	106.1	114.7	109.9	—	—
θ_1	B3LYP/TZ2P-ECP	—	114.8	112.9	115.0	112.1
θ_1	BLYP/TZ2P-ECP	—	113.8	111.7	113.4	110.4
θ_2	B3LYP/DZP	122.3	125.1	122.2	—	—
θ_2	BLYP/DZP	122.4	125.4	122.6	—	—
θ_2	B3LYP/DZP-ECP	—	123.7	122.7	121.8	116.7
θ_2	BLYP/DZP-ECP	—	124.0	122.9	121.8	116.5
θ_2	B3LYP/TZ2P	122.4	125.2	122.2	—	—
θ_2	BLYP/TZ2P	122.5	125.6	122.5	—	—

θ_2	B3LYP/TZ2P-ECP	—	124.2	122.9	122.2	115.8
θ_2	BLYP/TZ2P-ECP	—	124.5	123.1	122.2	115.8
θ_3	B3LYP/DZP	126.2	128.8	132.8	—	—
θ_3	BLYP/DZP	126.5	129.0	133.1	—	—
θ_3	B3LYP/DZP-ECP	—	130.2	133.0	137.2	146.3
θ_3	BLYP/DZP-ECP	—	130.4	133.3	137.7	146.8
θ_3	B3LYP/TZ2P	126.0	128.2	132.6	—	—
θ_3	BLYP/TZ2P	126.3	128.3	132.9	—	—
θ_3	B3LYP/TZ2P-ECP	—	129.4	131.7	135.9	147.4
θ_3	BLYP/TZ2P-ECP	—	129.5	132.0	136.3	147.7
θ_4	B3LYP/DZP	109.4	110.6	109.8	—	—
θ_4	BLYP/DZP	109.4	110.5	109.5	—	—
θ_4	B3LYP/DZP-ECP	—	110.4	110.3	110.6	110.2
θ_4	BLYP/DZP-ECP	—	110.3	110.0	110.4	109.6
θ_4	B3LYP/TZ2P	109.6	110.2	109.3	—	—
θ_4	BLYP/TZ2P	109.5	110.1	109.0	—	—
θ_4	B3LYP/TZ2P-ECP	—	109.9	109.5	110.0	110.0
θ_4	BLYP/TZ2P-ECP	—	109.8	109.3	109.7	109.4
θ_5	B3LYP/DZP	109.7	110.3	108.8	—	—
θ_5	BLYP/DZP	109.9	110.3	108.6	—	—
θ_5	B3LYP/DZP-ECP	—	110.1	109.0	108.6	106.7
θ_5	BLYP/DZP-ECP	—	110.1	108.9	108.3	106.3
θ_5	B3LYP/TZ2P	109.8	110.0	108.7	—	—
θ_5	BLYP/TZ2P	110.0	110.0	108.4	—	—
θ_5	B3LYP/TZ2P-ECP	—	109.8	109.0	108.5	106.4
θ_5	BLYP/TZ2P-ECP	—	109.8	109.0	108.3	106.0
θ_6	B3LYP/DZP	107.6	107.3	108.8	—	—
θ_6	BLYP/DZP	107.5	107.4	109.1	—	—
θ_6	B3LYP/DZP-ECP	—	107.7	108.6	108.9	110.1
θ_6	BLYP/DZP-ECP	—	107.8	108.8	109.3	110.7
θ_6	B3LYP/TZ2P	107.4	107.5	109.0	—	—
θ_6	BLYP/TZ2P	107.3	107.6	109.4	—	—
θ_6	B3LYP/TZ2P-ECP	—	108.0	108.7	109.1	110.4
θ_6	BLYP/TZ2P-ECP	—	108.0	108.9	109.3	110.9

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Table VIII. A comparison of the geometric parameters for the group 14 congeners of the hydroperoxymethylcarbene molecule represented in Figure 4. Bond lengths are in angstroms and angles in degrees. Note that the carbon congener (X = C) has C_1 symmetry. The C-O-O-H torsion angle is approximately -12.0 degrees.

Parameter	Method/Basis	X = C	X = Si	X = Ge	X = Sn	X = Pb
r_1	B3LYP/DZP	0.973	0.973	0.973	—	—
r_1	BLYP/DZP	0.984	0.985	0.985	—	—
r_1	B3LYP/DZP-ECP	—	0.973	0.973	0.972	0.972
r_1	BLYP/DZP-ECP	—	0.985	0.985	0.984	0.984
r_1	B3LYP/TZ2P	0.963	0.966	0.965	—	—
r_1	BLYP/TZ2P	0.975	0.977	0.976	—	—
r_1	B3LYP/TZ2P-ECP	—	0.965	0.965	0.964	0.964
r_1	BLYP/TZ2P-ECP	—	0.976	0.976	0.975	0.975
r_2	B3LYP/DZP	1.887	1.479	1.465	—	—
r_2	BLYP/DZP	1.941	1.558	1.512	—	—
r_2	B3LYP/DZP-ECP	—	1.479	1.466	1.463	1.461
r_2	BLYP/DZP-ECP	—	1.559	1.517	1.503	1.496
r_2	B3LYP/TZ2P	1.974	1.485	1.469	—	—
r_2	BLYP/TZ2P	2.012	1.590	1.523	—	—
r_2	B3LYP/TZ2P-ECP	—	1.485	1.471	1.467	1.465
r_2	BLYP/TZ2P-ECP	—	1.592	1.532	1.514	1.505
r_3	B3LYP/DZP	1.186	1.678	1.820	—	—
r_3	BLYP/DZP	1.200	1.676	1.836	—	—
r_3	B3LYP/DZP-ECP	—	1.696	1.813	1.976	2.060
r_3	BLYP/DZP-ECP	—	1.690	1.822	1.992	2.081
r_3	B3LYP/TZ2P	1.159	1.672	1.826	—	—
r_3	BLYP/TZ2P	1.175	1.662	1.841	—	—
r_3	B3LYP/TZ2P-ECP	—	1.689	1.810	1.978	2.060
r_3	BLYP/TZ2P-ECP	—	1.677	1.817	1.993	2.082
r_4	B3LYP/DZP	1.486	1.901	2.000	—	—
r_4	BLYP/DZP	1.496	1.916	2.024	—	—
r_4	B3LYP/DZP-ECP	—	1.913	2.013	2.185	2.253
r_4	BLYP/DZP-ECP	—	1.926	2.030	2.202	2.273

r ₄	B3LYP/TZ2P	1.470	1.897	2.002	—	—
r ₄	BLYP/TZ2P	1.480	1.912	2.027	—	—
r ₄	B3LYP/TZ2P-ECP	—	1.900	2.000	2.178	2.249
r ₄	BLYP/TZ2P-ECP	—	1.915	2.019	2.198	2.271
r ₅	B3LYP/DZP	1.093	1.097	1.096	—	—
r ₅	BLYP/DZP	1.100	1.104	1.103	—	—
r ₅	B3LYP/DZP-ECP	—	1.095	1.096	1.096	1.097
r ₅	BLYP/DZP-ECP	—	1.102	1.103	1.103	1.104
r ₅	B3LYP/TZ2P	1.086	1.090	1.089	—	—
r ₅	BLYP/TZ2P	1.092	1.096	1.095	—	—
r ₅	B3LYP/TZ2P-ECP	—	1.087	1.088	1.089	1.089
r ₅	BLYP/TZ2P-ECP	—	1.090	1.094	1.095	1.095
r ₆	B3LYP/DZP	1.099	1.100	1.0983	—	—
r ₆	BLYP/DZP	1.106	1.107	1.105	—	—
r ₆	B3LYP/DZP-ECP	—	1.099	1.098	1.098	1.097
r ₆	BLYP/DZP-ECP	—	1.106	1.105	1.105	1.104
r ₆	B3LYP/TZ2P	1.091	1.093	1.091	—	—
r ₆	BLYP/TZ2P	1.073	1.099	1.097	—	—
r ₆	B3LYP/TZ2P-ECP	—	1.091	1.090	1.091	1.090
r ₆	BLYP/TZ2P-ECP	—	1.097	1.097	1.097	1.096
θ ₁	B3LYP/DZP	92.8	98.1	98.6	—	—
θ ₁	BLYP/DZP	91.4	96.0	97.2	—	—
θ ₁	B3LYP/DZP-ECP	—	98.0	98.4	98.7	98.9
θ ₁	BLYP/DZP-ECP	—	95.9	96.9	97.5	97.7
θ ₁	B3LYP/TZ2P	93.1	98.4	98.9	—	—
θ ₁	BLYP/TZ2P	91.9	95.8	97.4	—	—
θ ₁	B3LYP/TZ2P-ECP	—	98.4	98.9	99.2	99.3
θ ₁	BLYP/TZ2P-ECP	—	95.8	97.2	97.8	98.0
θ ₂	B3LYP/DZP	114.2	120.2	117.7	—	—
θ ₂	BLYP/DZP	114.7	121.0	118.2	—	—
θ ₂	B3LYP/DZP-ECP	—	119.1	118.6	117.6	116.5
θ ₂	BLYP/DZP-ECP	—	120.0	119.4	118.3	117.0

θ_2	B3LYP/TZ2P	111.7	120.1	117.6	—	—
θ_2	BLYP/TZ2P	112.8	121.1	118.2	—	—
θ_2	B3LYP/TZ2P-ECP	—	119.0	118.0	116.8	115.7
θ_2	BLYP/TZ2P-ECP	—	119.9	118.9	117.4	116.1
θ_3	B3LYP/DZP	129.6	102.9	100.1	—	—
θ_3	BLYP/DZP	129.4	104.8	101.0	—	—
θ_3	B3LYP/DZP-ECP	—	102.2	99.8	97.9	97.5
θ_3	BLYP/DZP-ECP	—	104.1	101.0	98.9	98.5
θ_3	B3LYP/TZ2P	133.4	103.2	100.2	—	—
θ_3	BLYP/TZ2P	132.6	105.7	101.2	—	—
θ_3	B3LYP/TZ2P-ECP	—	102.7	100.1	98.1	97.6
θ_3	BLYP/TZ2P-ECP	—	105.3	101.4	99.2	98.6
θ_4	B3LYP/DZP	106.9	110.9	110.0	—	—
θ_4	BLYP/DZP	106.6	110.4	109.8	—	—
θ_4	B3LYP/DZP-ECP	—	110.7	110.2	110.0	109.5
θ_4	BLYP/DZP-ECP	—	110.2	110.1	110.0	109.5
θ_4	B3LYP/TZ2P	105.9	110.4	109.8	—	—
θ_4	BLYP/TZ2P	106.2	109.8	109.7	—	—
θ_4	B3LYP/TZ2P-ECP	—	110.3	110.1	109.9	109.4
θ_4	BLYP/TZ2P-ECP	—	109.7	109.9	109.9	109.4
θ_5	B3LYP/DZP	111.3	111.1	110.7	—	—
θ_5	BLYP/DZP	111.6	111.4	110.6	—	—
θ_5	B3LYP/DZP-ECP	—	110.8	110.9	111.6	111.6
θ_5	BLYP/DZP-ECP	—	111.2	110.9	111.5	111.4
θ_5	B3LYP/TZ2P	111.4	110.9	110.3	—	—
θ_5	BLYP/TZ2P	111.8	111.3	110.2	—	—
θ_5	B3LYP/TZ2P-ECP	—	110.6	110.6	111.3	111.2
θ_5	BLYP/TZ2P-ECP	—	111.0	110.6	111.1	110.9
θ_6	B3LYP/DZP	109.4	106.3	107.0	—	—
θ_6	BLYP/DZP	109.2	106.5	107.3	—	—
θ_6	B3LYP/DZP-ECP	—	106.3	106.6	106.7	107.2
θ_6	BLYP/DZP-ECP	—	106.5	106.8	106.9	107.4
θ_6	B3LYP/TZ2P	110.0	106.9	107.4	—	—
θ_6	BLYP/TZ2P	109.4	107.2	107.7	—	—
θ_6	B3LYP/TZ2P-ECP	—	106.9	107.0	107.1	107.6
θ_6	BLYP/TZ2P-ECP	—	107.2	107.3	107.3	107.8