

Systematic study of the performance of density functional theory methods for prediction of energies and geometries of organoselenium compounds

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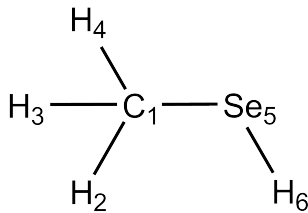
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S1 – MeSeH



S1a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,3)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,4)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,5)	2.026	1.9908	1.9917	1.992	2.0244	2.0024	2.0062	2.0056	1.9948	1.9988	1.9963	1.9983	1.9977
A(2,1,3)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(2,1,4)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(2,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
A(3,1,4)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(3,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
A(4,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
D(2,1,4,3)	117.7836	115.308	116.9619	117.2753	117.608	116.7091	117.7811	117.753	116.5898	117.7739	116.9091	117.9328	117.8943
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2439.07754623	-2439.3033521	-2439.34802684	-2439.34911541	-2441.47261186	-2441.50543794	-2441.51506562	-2441.51517671	-2441.5064637	-2441.51611731	-2441.51275223	-2441.52155076	-2441.52167796
ZPE Correction	0.035798	0.035551	0.035817	0.035643	0.03566	0.035342	0.035482	0.035446	0.035336	0.035497	0.035358	0.035521	0.035493

S1b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0886	1.0889	1.0898	1.0898	1.0856	1.0878	1.0879	1.0879	1.0868	1.0869	1.0853	1.0853	1.0853
R(1,3)	1.0886	1.0889	1.0898	1.0898	1.0856	1.0878	1.0879	1.0879	1.0868	1.0869	1.0853	1.0853	1.0853
R(1,4)	1.0903	1.0904	1.0913	1.0912	1.0869	1.0894	1.0895	1.0895	1.0885	1.0885	1.087	1.087	1.087
R(1,5)	1.9857	1.9515	1.9436	1.9461	1.9763	1.9584	1.9582	1.9583	1.9513	1.9512	1.9512	1.9512	1.9513
R(5,6)	1.4769	1.4578	1.4588	1.4612	1.4826	1.4681	1.4682	1.4682	1.467	1.4671	1.4666	1.4666	1.4666
A(2,1,3)	111.6171	111.2567	110.5977	110.8797	110.6737	110.9591	110.9488	110.9515	110.8915	110.8897	110.9188	110.9432	110.9461
A(2,1,4)	109.6992	109.3346	109.045	109.1441	109.2753	109.3439	109.3433	109.3509	109.3378	109.3401	109.3743	109.3931	109.395
A(2,1,5)	109.7516	110.4077	111.013	110.8747	110.5918	110.5797	110.5876	110.5771	110.6093	110.6118	110.5779	110.5556	110.553
A(3,1,4)	109.6965	109.3317	109.0423	109.1408	109.2726	109.3409	109.3404	109.348	109.3349	109.3372	109.3713	109.3901	109.392
A(3,1,5)	109.7522	110.4056	111.0097	110.8714	110.5897	110.5767	110.5844	110.5739	110.6059	110.6083	110.5742	110.5519	110.5493
A(4,1,5)	106.1765	105.9553	105.9936	105.7761	106.3274	105.9022	105.8982	105.9017	105.9269	105.919	105.8886	105.8702	105.8685
A(1,5,6)	94.2217	95.1671	95.8379	95.6843	94.8881	95.1796	95.2013	95.2061	95.4149	95.4429	95.4653	95.4894	95.4897
D(2,1,5,6)	-61.5326	-61.7499	-61.7664	-61.8566	-61.5116	-61.6836	-61.6829	-61.6771	-61.6627	-61.6633	-61.6595	-61.6596	-61.6597
D(3,1,5,6)	61.4808	61.6948	61.6851	61.7605	61.446	61.6202	61.6186	61.6133	61.5958	61.5963	61.5899	61.5899	61.5899
D(4,1,5,6)	-180.0274	179.9702	179.9568	179.9492	-180.035	179.9658	179.9653	179.9655	179.9639	179.9638	179.9625	179.9624	179.9623
Energy	-2440.61884766	-2440.85577794	-2440.87330719	-2440.87428455	-2442.99735547	-2443.03952596	-2443.0399135	-2443.0400106	-2443.04142167	-2443.0418482	-2443.04717754	-2443.04747963	-2443.0475132
ZPE Correction	0.044987	0.044937	0.044779	0.044585	0.044639	0.044362	0.044341	0.044345	0.044332	0.044324	0.044342	0.044335	0.044333

S1c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0894	1.0896	1.0905	1.0905	1.0864	1.0886	1.0887	1.0887	1.0876	1.0877	1.0862	1.0862	1.0862
R(1,3)	1.0894	1.0896	1.0905	1.0905	1.0864	1.0886	1.0887	1.0887	1.0876	1.0877	1.0862	1.0862	1.0862
R(1,4)	1.091	1.091	1.092	1.0919	1.0877	1.0901	1.0902	1.0902	1.0893	1.0893	1.0879	1.0879	1.0879
R(1,5)	1.9889	1.9545	1.9464	1.949	1.9797	1.9614	1.9613	1.9614	1.9544	1.9543	1.9542	1.9543	1.9544
R(5,6)	1.4783	1.4591	1.4601	1.4625	1.4846	1.4699	1.47	1.47	1.4688	1.4689	1.4685	1.4685	1.4685
A(2,1,3)	111.6306	111.2491	110.5903	110.8722	110.6869	110.9578	110.9472	110.9504	110.8937	110.8918	110.9159	110.9429	110.9461
A(2,1,4)	109.7251	109.3436	109.0564	109.158	109.3045	109.3574	109.3561	109.3632	109.3522	109.3548	109.3825	109.4034	109.4055
A(2,1,5)	109.72	110.3952	110.997	110.8544	110.5625	110.5645	110.5727	110.5632	110.5925	110.5945	110.566	110.5415	110.5387
A(3,1,4)	109.7224	109.3407	109.0536	109.1548	109.3018	109.3545	109.3532	109.3602	109.3492	109.3519	109.3795	109.4004	109.4025
A(3,1,5)	109.7205	110.3932	110.9937	110.8511	110.5604	110.5615	110.5696	110.56	110.589	110.591	110.5623	110.5379	110.5351
A(4,1,5)	106.1737	105.9714	106.0125	105.7989	106.3146	105.9078	105.9049	105.9071	105.9306	105.9229	105.9	105.879	105.877
A(1,5,6)	94.2095	95.164	95.8332	95.6787	94.894	95.1739	95.1957	95.2021	95.4052	95.4363	95.4505	95.479	95.4792
D(2,1,5,6)	-61.5203	-61.7368	-61.7507	-61.8374	-61.5006	-61.6724	-61.6717	-61.6668	-61.6524	-61.6526	-61.6493	-61.6496	-61.6498
D(3,1,5,6)	61.4683	61.681	61.6684	61.7411	61.4335	61.6086	61.6072	61.6028	61.5854	61.5856	61.5799	61.58	61.58
D(4,1,5,6)	-180.0275	179.9699	179.9563	179.9491	-180.0357	179.9655	179.9652	179.9654	179.9638	179.9639	179.9626	179.9625	179.9624
Energy	-2439.62263094	-2439.8596044	-2439.8772367	-2439.87822219	-2441.99820744	-2442.04038332	-2442.04084238	-2442.04094456	-2442.04214854	-2442.04265494	-2442.04789423	-2442.04824963	-2442.0482841
ZPE Correction	0.044925	0.044873	0.044718	0.044526	0.044574	0.044295	0.044272	0.044274	0.044259	0.04425	0.044265	0.044257	0.044254

S1d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0959	1.0963	1.0969	1.0969	1.0932	1.0949	1.095	1.095	1.0939	1.094	1.0924	1.0924	1.0924
R(1,3)	1.0959	1.0963	1.0969	1.0969	1.0932	1.0949	1.095	1.095	1.0939	1.094	1.0924	1.0924	1.0924
R(1,4)	1.0971	1.0974	1.098	1.098	1.0942	1.0961	1.0963	1.0963	1.0952	1.0953	1.0938	1.0938	1.0938
R(1,5)	2.0307	1.9878	1.9797	1.9833	2.0175	1.9953	1.9955	1.9956	1.9877	1.9879	1.987	1.9873	1.9873
R(5,6)	1.4877	1.4658	1.4673	1.47	1.4946	1.4772	1.4774	1.4774	1.4757	1.4759	1.4751	1.4751	1.4751
A(2,1,3)	111.931	111.3458	110.7337	111.0852	110.9078	111.0667	111.0682	111.0709	111.0115	111.0212	111.0215	111.0635	111.0664
A(2,1,4)	110.2008	109.614	109.3472	109.4753	109.6645	109.6483	109.6547	109.6615	109.6404	109.6554	109.6644	109.6986	109.7002
A(2,1,5)	109.1991	110.0908	110.6737	110.4693	110.1671	110.2334	110.2377	110.2295	110.2546	110.2463	110.2435	110.2031	110.2016
A(3,1,4)	110.1998	109.6113	109.3457	109.4733	109.6622	109.6456	109.6521	109.6589	109.6377	109.6528	109.6617	109.6959	109.6975
A(3,1,5)	109.199	110.088	110.6713	110.4666	110.1644	110.2297	110.2341	110.2258	110.2506	110.2424	110.2393	110.199	110.1975
A(4,1,5)	105.9223	105.9461	105.9424	105.7241	106.1622	105.8845	105.8604	105.8606	105.9174	105.8929	105.8802	105.8477	105.8444
A(1,5,6)	93.3992	94.5484	95.2052	95.0249	94.1561	94.5347	94.5668	94.5735	94.7545	94.7894	94.8025	94.8351	94.8361
D(2,1,5,6)	-61.3517	-61.5851	-61.5995	-61.688	-61.3682	-61.5113	-61.5149	-61.5114	-61.4911	-61.4909	-61.4907	-61.4894	-61.4905
D(3,1,5,6)	61.3342	61.5387	61.5482	61.6233	61.3066	61.4526	61.4568	61.4526	61.4318	61.4329	61.4296	61.4293	61.4298
D(4,1,5,6)	-180.0093	179.9745	179.9728	179.9657	179.9671	-180.0319	-180.0316	-180.032	-180.0323	-180.0316	-180.0332	-180.0327	-180.033
Energy	-2440.83787823	-2441.06700073	-2441.0855163	-2441.08657812	-2443.19798906	-2443.23817092	-2443.23884686	-2443.23892125	-2443.24025155	-2443.24097873	-2443.24516731	-2443.24568923	-2443.24571787
ZPE Correction	0.043507	0.043418	0.043224	0.043016	0.043169	0.04293	0.042902	0.042897	0.042897	0.042886	0.042902	0.042891	0.042887

S1e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0906	1.0911	1.0921	1.092	1.0876	1.0898	1.0899	1.0898	1.0888	1.0889	1.0873	1.0873	1.0873
R(1,3)	1.0906	1.0911	1.0921	1.092	1.0876	1.0898	1.0899	1.0898	1.0888	1.0889	1.0873	1.0873	1.0873
R(1,4)	1.092	1.0926	1.0936	1.0936	1.089	1.0914	1.0915	1.0915	1.0906	1.0907	1.0891	1.0891	1.0891
R(1,5)	2.0005	1.9655	1.9575	1.9603	1.9893	1.9718	1.9718	1.9719	1.9649	1.965	1.9649	1.9651	1.9651
R(5,6)	1.4789	1.4603	1.4614	1.4639	1.4859	1.4717	1.4718	1.4718	1.4706	1.4708	1.4704	1.4704	1.4704
A(2,1,3)	111.7621	111.3334	110.6826	110.9789	110.7854	111.0461	111.0434	111.0456	110.9921	110.9959	111.0085	111.0386	111.0412
A(2,1,4)	109.8912	109.4791	109.1942	109.2938	109.4332	109.4853	109.4874	109.4944	109.4836	109.491	109.5136	109.5385	109.5397
A(2,1,5)	109.5437	110.2389	110.8509	110.7015	110.4183	110.4086	110.4151	110.4067	110.4331	110.4322	110.4074	110.3793	110.3779
A(3,1,4)	109.8899	109.4763	109.1915	109.2906	109.4305	109.4824	109.4846	109.4916	109.4808	109.4882	109.5108	109.5358	109.5369
A(3,1,5)	109.5438	110.2369	110.8476	110.6983	110.4162	110.4056	110.412	110.4035	110.4297	110.4288	110.4039	110.3758	110.3744
A(4,1,5)	106.047	105.9275	105.9399	105.7268	106.2464	105.8758	105.8606	105.8615	105.8875	105.8698	105.8616	105.8361	105.8339
A(1,5,6)	94.1258	95.0848	95.7692	95.6139	94.8209	95.0679	95.0972	95.1034	95.3033	95.3419	95.337	95.3712	95.3723
D(2,1,5,6)	-61.4723	-61.6817	-61.7062	-61.7978	-61.463	-61.6185	-61.6217	-61.6175	-61.6013	-61.6032	-61.595	-61.5951	-61.596
D(3,1,5,6)	61.4486	61.6283	61.6241	61.7014	61.398	61.5592	61.5615	61.5569	61.5412	61.543	61.5329	61.5325	61.5329
D(4,1,5,6)	-180.0125	179.9711	179.9564	179.9491	-180.0346	-180.0322	-180.0326	-180.0328	179.9674	179.9674	179.9664	179.9661	179.9659
Energy	-2439.46482887	-2439.70060028	-2439.71866489	-2439.71968725	-2441.84460854	-2441.88664517	-2441.88716653	-2441.88723904	-2441.88831259	-2441.88888146	-2441.89398048	-2441.89440298	-2441.89443165
ZPE Correction	0.044745	0.044704	0.044533	0.044334	0.044412	0.044142	0.044116	0.044114	0.044116	0.044104	0.044117	0.044108	0.044105

S1f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0898	1.0904	1.0914	1.0914	1.0868	1.0892	1.0893	1.0893	1.0884	1.0886	1.0876	1.0875	1.0875
R(1,3)	1.0898	1.0904	1.0914	1.0914	1.0868	1.0892	1.0893	1.0893	1.0884	1.0886	1.0876	1.0875	1.0875
R(1,4)	1.0911	1.0915	1.0926	1.0925	1.0881	1.0906	1.0908	1.0908	1.09	1.0902	1.0892	1.0891	1.0891
R(1,5)	1.9959	1.9543	1.9469	1.9495	1.9857	1.9644	1.9648	1.9649	1.9574	1.9578	1.9566	1.9572	1.9572
R(5,6)	1.4804	1.4596	1.4609	1.4634	1.4899	1.4722	1.4725	1.4726	1.4704	1.4707	1.4705	1.4706	1.4707
A(2,1,3)	111.6764	111.1091	110.4551	110.7545	110.708	110.8983	110.91	110.9096	110.845	110.8636	110.8274	110.8621	110.867
A(2,1,4)	109.759	109.1963	108.9139	109.0023	109.3191	109.2808	109.2936	109.2957	109.2728	109.2983	109.2777	109.3178	109.3152
A(2,1,5)	109.7317	110.6083	111.2023	111.0799	110.597	110.6846	110.6867	110.6855	110.7146	110.6999	110.7277	110.6872	110.6903
A(3,1,4)	109.7578	109.1932	108.9109	108.9988	109.3164	109.2776	109.2905	109.2926	109.2696	109.2952	109.2745	109.3146	109.312
A(3,1,5)	109.7317	110.6059	111.1986	111.0762	110.5946	110.6812	110.6832	110.6819	110.7108	110.6961	110.7238	110.6833	110.6864
A(4,1,5)	106.0262	105.9793	106.0146	105.7682	106.1901	105.8779	105.8343	105.8332	105.89	105.8482	105.8718	105.8369	105.8304
A(1,5,6)	94.0238	95.0186	95.7137	95.5646	94.8731	95.0879	95.1399	95.146	95.3219	95.3815	95.3422	95.3992	95.4034
D(2,1,5,6)	-61.5405	-61.7952	-61.8102	-61.9244	-61.5342	-61.7152	-61.7245	-61.7249	-61.7005	-61.7019	-61.6995	-61.694	-61.7002
D(3,1,5,6)	61.5205	61.7404	61.7289	61.825	61.4741	61.6571	61.6657	61.663	61.6455	61.6473	61.6422	61.6354	61.6398
D(4,1,5,6)	-180.0107	179.9701	179.9566	179.9472	-180.0323	179.9681	179.9678	179.9662	179.9696	179.9698	179.9684	179.9677	179.9668
Energy	-2440.95700186	-2441.18840149	-2441.20759231	-2441.20863471	-2443.31597816	-2443.35834157	-2443.35930716	-2443.35934645	-2443.35986419	-2443.36088531	-2443.36495578	-2443.36567021	-2443.36570965
ZPE Correction	0.044427	0.044344	0.044133	0.04391	0.044084	0.043759	0.043716	0.043699	0.043672	0.04365	0.043651	0.043636	0.04363

S1g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0891	1.0897	1.0907	1.0907	1.0862	1.0886	1.0888	1.0888	1.0879	1.088	1.0869	1.0868	1.0869
R(1,3)	1.0891	1.0897	1.0907	1.0907	1.0862	1.0886	1.0888	1.0888	1.0879	1.088	1.0869	1.0868	1.0869
R(1,4)	1.0904	1.0909	1.092	1.0919	1.0875	1.0901	1.0903	1.0904	1.0894	1.0896	1.0885	1.0885	1.0885
R(1,5)	1.9943	1.9561	1.9484	1.9509	1.9839	1.9643	1.9646	1.9647	1.9576	1.9579	1.9571	1.9576	1.9576
R(5,6)	1.4767	1.4577	1.4587	1.4612	1.4859	1.4702	1.4704	1.4705	1.4687	1.4689	1.4689	1.4689	1.4689
A(2,1,3)	111.6652	111.1632	110.5133	110.7991	110.6952	110.9162	110.9236	110.9239	110.8685	110.8827	110.8544	110.8941	110.8978
A(2,1,4)	109.7804	109.2919	109.0134	109.1091	109.3446	109.3407	109.3487	109.3518	109.341	109.3595	109.3448	109.3826	109.3818
A(2,1,5)	109.6878	110.474	111.0607	110.9286	110.5522	110.5991	110.6002	110.5979	110.6217	110.61	110.6275	110.5864	110.5876
A(3,1,4)	109.7792	109.2892	109.0108	109.1062	109.3421	109.3379	109.3459	109.349	109.3382	109.3568	109.342	109.3799	109.379
A(3,1,5)	109.688	110.472	111.0574	110.9254	110.5501	110.5961	110.5971	110.5948	110.6183	110.6066	110.6239	110.5829	110.5841
A(4,1,5)	106.0858	106.0061	106.0487	105.8214	106.2453	105.915	105.8881	105.8863	105.9194	105.8904	105.9151	105.8802	105.8755
A(1,5,6)	94.1606	95.1139	95.7954	95.6456	94.9413	95.1396	95.1798	95.1888	95.376	95.4302	95.3919	95.4465	95.4493
D(2,1,5,6)	-61.5063	-61.7359	-61.7459	-61.843	-61.4972	-61.6675	-61.6727	-61.6722	-61.6527	-61.6531	-61.6484	-61.6452	-61.6489
D(3,1,5,6)	61.4828	61.6817	61.6651	61.7473	61.4331	61.6085	61.6142	61.6119	61.5938	61.5952	61.588	61.5847	61.5873
D(4,1,5,6)	-180.0124	179.9707	179.9572	179.9495	-180.0341	179.968	179.9683	179.9673	179.968	179.9686	179.9673	179.9672	179.9667
Energy	-2440.11887052	-2440.35265365	-2440.37165166	-2440.37267323	-2442.49067908	-2442.53334843	-2442.53433392	-2442.53439931	-2442.53471335	-2442.53577112	-2442.54016965	-2442.54092159	-2442.54095761
ZPE Correction	0.044762	0.044701	0.0445	0.044285	0.044418	0.044111	0.04407	0.044056	0.044041	0.044021	0.044019	0.044005	0.043998

S1h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.097	1.0972	1.0984	1.0984	1.0941	1.0959	1.096	1.096	1.0949	1.0951	1.0936	1.0936	1.0936
R(1,3)	1.097	1.0972	1.0984	1.0984	1.0941	1.0959	1.096	1.096	1.0949	1.0951	1.0936	1.0936	1.0936
R(1,4)	1.0985	1.0987	1.0998	1.0998	1.0954	1.0974	1.0976	1.0976	1.0966	1.0968	1.0954	1.0953	1.0954
R(1,5)	2.0061	1.9683	1.9605	1.9634	1.9965	1.9763	1.9764	1.9765	1.969	1.9692	1.9687	1.969	1.969
R(5,6)	1.493	1.4713	1.4729	1.4755	1.5002	1.483	1.4832	1.4833	1.4814	1.4816	1.4813	1.4814	1.4814
A(2,1,3)	111.822	111.3564	110.6721	110.9906	110.825	111.0861	111.0828	111.0851	111.049	111.0553	111.06	111.0999	111.1024
A(2,1,4)	109.8248	109.3698	109.0666	109.1627	109.3488	109.3959	109.3969	109.4047	109.4148	109.4261	109.4436	109.4767	109.4774
A(2,1,5)	109.6558	110.4024	111.0355	110.885	110.5528	110.546	110.5578	110.5493	110.54	110.5379	110.5242	110.4866	110.4862
A(3,1,4)	109.8236	109.3668	109.0637	109.1593	109.3462	109.3929	109.394	109.4017	109.4118	109.4232	109.4406	109.4737	109.4744
A(3,1,5)	109.6558	110.4001	111.032	110.8815	110.5507	110.5428	110.5545	110.5459	110.5364	110.5343	110.5204	110.4828	110.4824
A(4,1,5)	105.8852	105.7837	105.8214	105.5942	106.0942	105.7266	105.7034	105.7029	105.7418	105.7159	105.7039	105.6709	105.6675
A(1,5,6)	93.8034	94.8129	95.5105	95.3504	94.5001	94.7368	94.7757	94.7831	94.9643	95.0116	95.0042	95.0475	95.0492
D(2,1,5,6)	-61.5801	-61.8068	-61.8288	-61.9343	-61.5783	-61.7373	-61.7435	-61.7396	-61.7088	-61.7112	-61.7061	-61.7056	-61.7072
D(3,1,5,6)	61.5626	61.7573	61.7506	61.8399	61.5179	61.6813	61.6872	61.6822	61.654	61.6567	61.6484	61.6476	61.6486
D(4,1,5,6)	-180.0094	179.9729	179.9582	179.9499	-180.0324	-180.0306	-180.0307	-180.0313	-180.0301	-180.0299	-180.0316	-180.0317	-180.032
Energy	-2439.20056008	-2439.43790408	-2439.45674599	-2439.45780789	-2441.57073232	-2441.61296859	-2441.61371074	-2441.61378202	-2441.61468793	-2441.61548436	-2441.62010445	-2441.62068623	-2441.62071791
ZPE Correction	0.043711	0.04357	0.043392	0.043194	0.043388	0.043058	0.043025	0.043019	0.043022	0.043007	0.043025	0.043013	0.043009

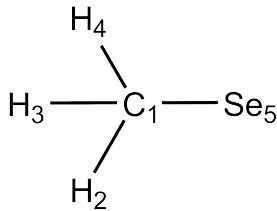
S1i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0912	1.0916	1.0926	1.0925	1.0881	1.0901	1.0902	1.0902	1.089	1.0891	1.0874	1.0874	1.0874
R(1,3)	1.0912	1.0916	1.0926	1.0925	1.0881	1.0901	1.0902	1.0902	1.089	1.0891	1.0874	1.0874	1.0874
R(1,4)	1.0925	1.093	1.094	1.0939	1.0894	1.0916	1.0917	1.0917	1.0907	1.0907	1.0891	1.0891	1.0891
R(1,5)	1.9995	1.9633	1.9553	1.958	1.9877	1.9696	1.9695	1.9696	1.9628	1.9627	1.9625	1.9627	1.9627
R(5,6)	1.4795	1.4598	1.4609	1.4634	1.4854	1.4705	1.4706	1.4706	1.4694	1.4695	1.4687	1.4688	1.4688
A(2,1,3)	111.7792	111.3314	110.6699	110.9649	110.8016	111.0552	111.0463	111.0497	110.9985	110.9978	111.014	111.0446	111.0476
A(2,1,4)	109.8905	109.4682	109.1804	109.2809	109.4342	109.4873	109.4871	109.4945	109.4887	109.4934	109.5177	109.5411	109.5431
A(2,1,5)	109.5555	110.2732	110.8895	110.7409	110.4332	110.4284	110.4377	110.4283	110.4449	110.4463	110.4244	110.3965	110.3942
A(3,1,4)	109.8893	109.4655	109.1778	109.2779	109.4316	109.4845	109.4843	109.4917	109.486	109.4907	109.515	109.5384	109.5404
A(3,1,5)	109.5557	110.2712	110.8863	110.7377	110.4312	110.4255	110.4347	110.4253	110.4416	110.443	110.421	110.3931	110.3908
A(4,1,5)	106.0046	105.88	105.9002	105.6851	106.1954	105.8196	105.8105	105.8112	105.8448	105.8329	105.8112	105.7878	105.7853
A(1,5,6)	94.0231	95.0145	95.6947	95.5399	94.7652	95.0455	95.071	95.0788	95.2707	95.3026	95.312	95.3399	95.3408
D(2,1,5,6)	-61.4901	-61.7035	-61.7246	-61.8158	-61.4837	-61.6393	-61.6403	-61.6359	-61.6146	-61.6151	-61.612	-61.6123	-61.6127
D(3,1,5,6)	61.4675	61.6508	61.6441	61.7211	61.4182	61.5773	61.5777	61.5735	61.5524	61.5531	61.5464	61.5467	61.5468
D(4,1,5,6)	-180.012	179.9715	179.9573	179.95	-180.0349	-180.0334	-180.0337	-180.0336	-180.0336	-180.0334	179.9648	179.9648	179.9646
Energy	-2439.80192093	-2440.03709128	-2440.05499208	-2440.05600027	-2442.17348596	-2442.21447546	-2442.21496331	-2442.21505504	-2442.21653548	-2442.21706843	-2442.22215573	-2442.22253704	-2442.22256606
ZPE Correction	0.044564	0.044524	0.04436	0.044164	0.044225	0.043972	0.043948	0.043948	0.043951	0.043941	0.043962	0.043955	0.043951

S1j – QCISD

	QCISD/cc-pVTZ
R(1,2)	1.0853
R(1,3)	1.0853
R(1,4)	1.0872
R(1,5)	1.9495
R(5,6)	1.4577
A(2,1,3)	110.7328
A(2,1,4)	109.2854
A(2,1,5)	110.6410
A(3,1,4)	109.2828
A(3,1,5)	110.6371
A(4,1,5)	106.1412
A(1,5,6)	95.3566
D(2,1,5,6)	-61.5855
D(3,1,5,6)	61.5144
D(4,1,5,6)	179.9619
Energy	-2440.5325151
ZPE Correction	0.045024

S2 – MeSe[−]



S2a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,3)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,4)	1.0979	1.0985	1.096	1.0963	1.0934	1.0953	1.0935	1.0936	1.0941	1.0922	1.0924	1.0905	1.0907
R(1,5)	2.026	1.9908	1.9917	1.992	2.0244	2.0024	2.0062	2.0056	1.9948	1.9988	1.9963	1.9983	1.9977
A(2,1,3)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(2,1,4)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(2,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
A(3,1,4)	108.538	107.4256	108.1772	108.3158	108.4616	108.0645	108.5369	108.5247	108.0111	108.5338	108.1538	108.6027	108.586
A(3,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
A(4,1,5)	110.3891	111.4467	110.7362	110.6033	110.4629	110.8437	110.3901	110.4019	110.8946	110.3931	110.7586	110.3264	110.3426
D(2,1,4,3)	117.7836	115.308	116.9619	117.2753	117.608	116.7091	117.7811	117.753	116.5898	117.7739	116.9091	117.9328	117.8943
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2439.07754623	-2439.3033521	-2439.34802684	-2439.34911541	-2441.47261186	-2441.50543794	-2441.51506562	-2441.51517671	-2441.5064637	-2441.51611731	-2441.51275223	-2441.52155076	-2441.52167796
ZPE Correction	0.035798	0.035551	0.035817	0.035643	0.03566	0.035342	0.035482	0.035446	0.035336	0.035497	0.035358	0.035521	0.035493

S2b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.097	1.098	1.0959	1.0962	1.0933	1.0954	1.0939	1.094	1.0943	1.0929	1.0928	1.0913	1.0915
R(1,3)	1.097	1.098	1.0959	1.0962	1.0933	1.0954	1.0939	1.094	1.0943	1.0929	1.0928	1.0913	1.0915
R(1,4)	1.097	1.098	1.0959	1.0962	1.0933	1.0954	1.0939	1.094	1.0943	1.0929	1.0928	1.0913	1.0915
R(1,5)	2.0082	1.9712	1.9698	1.9702	2.0057	1.9819	1.9842	1.9837	1.9746	1.9766	1.9755	1.9766	1.976
A(2,1,3)	108.604	107.3407	107.9034	108.058	108.4384	107.9252	108.2992	108.2878	107.8639	108.2628	107.9815	108.3522	108.333
A(2,1,4)	108.604	107.3407	107.9034	108.058	108.4384	107.9252	108.2992	108.2878	107.8639	108.2628	107.9815	108.3522	108.333
A(2,1,5)	110.3251	111.5258	110.9969	110.8499	110.4853	110.9762	110.6193	110.6302	111.0343	110.6541	110.9228	110.5683	110.5868
A(3,1,4)	108.604	107.3407	107.9034	108.058	108.4384	107.9252	108.2992	108.2878	107.8639	108.2628	107.9815	108.3522	108.333
A(3,1,5)	110.3251	111.5258	110.9969	110.8499	110.4853	110.9762	110.6193	110.6302	111.0343	110.6541	110.9228	110.5683	110.5868
A(4,1,5)	110.3251	111.5258	110.9969	110.8499	110.4853	110.9762	110.6193	110.6302	111.0343	110.6541	110.9228	110.5683	110.5868
D(2,1,4,3)	117.9359	115.126	116.3506	116.6945	117.5549	116.3989	117.2375	117.2118	116.2633	117.1552	116.5238	117.3582	117.3144
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2440.04212835	-2440.26711911	-2440.30646001	-2440.30750523	-2442.4364242	-2442.46932895	-2442.47665046	-2442.47675193	-2442.47039053	-2442.47773568	-2442.47636634	-2442.4830829	-2442.48320432
ZPE Correction	0.036009	0.035708	0.035965	0.035794	0.035873	0.035502	0.035621	0.035592	0.035474	0.035611	0.03549	0.035627	0.035605

S2c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0977	1.0986	1.0966	1.0969	1.0942	1.0962	1.0946	1.0948	1.0952	1.0937	1.0938	1.0922	1.0924
R(1,3)	1.0977	1.0986	1.0966	1.0969	1.0942	1.0962	1.0946	1.0948	1.0952	1.0937	1.0938	1.0922	1.0924
R(1,4)	1.0977	1.0986	1.0966	1.0969	1.0942	1.0962	1.0946	1.0948	1.0952	1.0937	1.0938	1.0922	1.0924
R(1,5)	2.0116	1.9745	1.9727	1.9732	2.0091	1.9852	1.9874	1.9869	1.9778	1.9798	1.9787	1.9797	1.9792
A(2,1,3)	108.626	107.3775	107.9377	108.0917	108.4468	107.9388	108.3164	108.3026	107.8792	108.2841	107.9941	108.3692	108.3495
A(2,1,4)	108.626	107.3775	107.9377	108.0917	108.4468	107.9388	108.3164	108.3026	107.8792	108.2841	107.9941	108.3692	108.3495
A(2,1,5)	110.3037	111.4916	110.9643	110.8178	110.4771	110.9633	110.6027	110.616	111.0198	110.6338	110.9108	110.552	110.5709
A(3,1,4)	108.626	107.3775	107.9377	108.0917	108.4468	107.9388	108.3164	108.3026	107.8792	108.2841	107.9941	108.3692	108.3495
A(3,1,5)	110.3037	111.4916	110.9643	110.8178	110.4771	110.9633	110.6027	110.616	111.0198	110.6338	110.9108	110.552	110.5709
A(4,1,5)	110.3037	111.4916	110.9643	110.8178	110.4771	110.9633	110.6027	110.616	111.0198	110.6338	110.9108	110.552	110.5709
D(2,1,4,3)	117.9869	115.2047	116.4266	116.7698	117.5742	116.4289	117.2768	117.2453	116.2971	117.2033	116.552	117.3967	117.352
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2439.04530099	-2439.27019989	-2439.30982541	-2439.3108229	-2441.43615188	-2441.46905694	-2441.47674668	-2441.47685345	-2441.47003326	-2441.4777479	-2441.47600144	-2441.48306458	-2441.48317806
ZPE Correction	0.03597	0.03567	0.035928	0.035753	0.035818	0.035453	0.035572	0.035538	0.035419	0.035558	0.035435	0.035574	0.035548

S2d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1065	1.1069	1.103	1.1035	1.1021	1.1034	1.1011	1.1013	1.1024	1.0999	1.1009	1.0985	1.0987
R(1,3)	1.1065	1.1069	1.103	1.1035	1.1021	1.1034	1.1011	1.1013	1.1024	1.0999	1.1009	1.0985	1.0987
R(1,4)	1.1065	1.1069	1.103	1.1035	1.1021	1.1034	1.1011	1.1013	1.1024	1.0999	1.1009	1.0985	1.0987
R(1,5)	2.0459	2.0098	2.0122	2.0121	2.044	2.0218	2.0255	2.0248	2.0138	2.0177	2.0145	2.0166	2.0159
A(2,1,3)	108.3858	107.279	108.2147	108.3324	108.3232	107.9384	108.4406	108.4261	107.8882	108.4533	108.0178	108.5071	108.4904
A(2,1,4)	108.3858	107.279	108.2147	108.3324	108.3232	107.9384	108.4406	108.4261	107.8882	108.4533	108.0178	108.5071	108.4904
A(2,1,5)	110.536	111.5834	110.7003	110.5874	110.5962	110.9637	110.4831	110.4971	111.0113	110.4709	110.8882	110.4189	110.4351
A(3,1,4)	108.3858	107.279	108.2147	108.3324	108.3232	107.9384	108.4406	108.4261	107.8882	108.4533	108.0178	108.5071	108.4904
A(3,1,5)	110.536	111.5834	110.7003	110.5874	110.5962	110.9637	110.4831	110.4971	111.0113	110.4709	110.8882	110.4189	110.4351
A(4,1,5)	110.536	111.5834	110.7003	110.5874	110.5962	110.9637	110.4831	110.4971	111.0113	110.4709	110.8882	110.4189	110.4351
D(2,1,4,3)	117.4346	114.9941	117.0464	117.3129	117.292	116.4281	117.56	117.5267	116.317	117.589	116.6047	117.7125	117.674
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2440.25298374	-2440.4722233	-2440.51755229	-2440.51859411	-2442.63174463	-2442.66397746	-2442.67427384	-2442.67438488	-2442.66529391	-2442.67561898	-2442.67075854	-2442.68005983	-2442.68017549
ZPE Correction	0.034655	0.034379	0.034741	0.034554	0.034551	0.034247	0.034424	0.034381	0.034213	0.034419	0.034227	0.034425	0.03439

S2e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0995	1.1002	1.098	1.0983	1.0956	1.0975	1.0958	1.096	1.0965	1.0948	1.0949	1.0932	1.0934
R(1,3)	1.0995	1.1002	1.098	1.0983	1.0956	1.0975	1.0958	1.096	1.0965	1.0948	1.0949	1.0932	1.0934
R(1,4)	1.0995	1.1002	1.098	1.0983	1.0956	1.0975	1.0958	1.096	1.0965	1.0948	1.0949	1.0932	1.0934
R(1,5)	2.0197	1.9839	1.9836	1.9842	2.0172	1.9946	1.9977	1.9971	1.9877	1.9906	1.9889	1.9905	1.9898
A(2,1,3)	108.6101	107.4539	108.0916	108.2443	108.4581	108.0064	108.4174	108.4029	107.9643	108.4077	108.0797	108.48	108.4597
A(2,1,4)	108.6101	107.4539	108.0916	108.2443	108.4581	108.0064	108.4174	108.4029	107.9643	108.4077	108.0797	108.48	108.4597
A(2,1,5)	110.3192	111.4202	110.8179	110.6719	110.4662	110.8991	110.5055	110.5195	110.9391	110.5149	110.8293	110.4451	110.4647
A(3,1,4)	108.6101	107.4539	108.0916	108.2443	108.4581	108.0064	108.4174	108.4029	107.9643	108.4077	108.0797	108.48	108.4597
A(3,1,5)	110.3192	111.4202	110.8179	110.6719	110.4662	110.8991	110.5055	110.5195	110.9391	110.5149	110.8293	110.4451	110.4647
A(4,1,5)	110.3192	111.4202	110.8179	110.6719	110.4662	110.8991	110.5055	110.5195	110.9391	110.5149	110.8293	110.4451	110.4647
D(2,1,4,3)	117.95	115.3689	116.7697	117.1132	117.6001	116.5792	117.5069	117.4736	116.4855	117.4846	116.743	117.6502	117.6037
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2438.88690021	-2439.11073489	-2439.15242113	-2439.15345312	-2441.2824634	-2441.31518658	-2441.32399586	-2441.32410682	-2441.31606659	-2441.32491378	-2441.32213579	-2441.33021045	-2441.33034079
ZPE Correction	0.035831	0.035558	0.035813	0.035642	0.035686	0.035344	0.035472	0.035437	0.035317	0.035467	0.035332	0.035483	0.035459

S2f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0993	1.1006	1.0972	1.0977	1.0952	1.0977	1.0953	1.0956	1.097	1.0946	1.0962	1.0936	1.0939
R(1,3)	1.0993	1.1006	1.0972	1.0977	1.0952	1.0977	1.0953	1.0956	1.097	1.0946	1.0962	1.0936	1.0939
R(1,4)	1.0993	1.1006	1.0972	1.0977	1.0952	1.0977	1.0953	1.0956	1.097	1.0946	1.0962	1.0936	1.0939
R(1,5)	2.015	1.9726	1.9745	1.9747	2.014	1.987	1.9925	1.9915	1.9794	1.9848	1.9797	1.9831	1.9821
A(2,1,3)	108.358	106.8901	107.7982	107.9307	108.2465	107.5645	108.2217	108.1852	107.5116	108.2054	107.607	108.2393	108.2057
A(2,1,4)	108.358	106.8901	107.7982	107.9307	108.2465	107.5645	108.2217	108.1852	107.5116	108.2054	107.607	108.2393	108.2057
A(2,1,5)	110.5627	111.9432	111.0965	110.971	110.6698	111.3165	110.6935	110.7285	111.3662	110.7092	111.2766	110.6767	110.7089
A(3,1,4)	108.358	106.8901	107.7982	107.9307	108.2465	107.5645	108.2217	108.1852	107.5116	108.2054	107.607	108.2393	108.2057
A(3,1,5)	110.5627	111.9432	111.0965	110.971	110.6698	111.3165	110.6935	110.7285	111.3662	110.7092	111.2766	110.6767	110.7089
A(4,1,5)	110.5627	111.9432	111.0965	110.971	110.6698	111.3165	110.6935	110.7285	111.3662	110.7092	111.2766	110.6767	110.7089
D(2,1,4,3)	117.3714	114.1744	116.1184	116.411	117.1183	115.6081	117.0623	116.98	115.4935	117.0254	115.7004	117.102	117.0261
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2440.37057066	-2440.59082186	-2440.63866039	-2440.63959381	-2442.74719858	-2442.7806189	-2442.79341682	-2442.79353121	-2442.78148889	-2442.79432297	-2442.78744361	-2442.79895993	-2442.79908964
ZPE Correction	0.03552	0.0352	0.035534	0.035333	0.035411	0.035016	0.035188	0.035134	0.03493	0.035136	0.034914	0.035132	0.035094

S2g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0981	1.0992	1.0966	1.0971	1.0945	1.0968	1.0949	1.0953	1.0961	1.0941	1.0951	1.093	1.0933
R(1,3)	1.0981	1.0992	1.0966	1.0971	1.0945	1.0968	1.0949	1.0953	1.0961	1.0941	1.0951	1.093	1.0933
R(1,4)	1.0981	1.0992	1.0966	1.0971	1.0945	1.0968	1.0949	1.0953	1.0961	1.0941	1.0951	1.093	1.0933
R(1,5)	2.014	1.9747	1.9741	1.9741	2.0113	1.9859	1.99	1.989	1.9788	1.9827	1.9795	1.9818	1.9809
A(2,1,3)	108.4874	107.1493	107.8593	107.9837	108.3007	107.6965	108.225	108.1884	107.6486	108.2117	107.7474	108.2601	108.2267
A(2,1,4)	108.4874	107.1493	107.8593	107.9837	108.3007	107.6965	108.225	108.1884	107.6486	108.2117	107.7474	108.2601	108.2267
A(2,1,5)	110.438	111.7038	111.0386	110.9206	110.6178	111.1925	110.6904	110.7254	111.2375	110.7031	111.1445	110.6567	110.6887
A(3,1,4)	108.4874	107.1493	107.8593	107.9837	108.3007	107.6965	108.225	108.1884	107.6486	108.2117	107.7474	108.2601	108.2267
A(3,1,5)	110.438	111.7038	111.0386	110.9206	110.6178	111.1925	110.6904	110.7254	111.2375	110.7031	111.1445	110.6567	110.6887
A(4,1,5)	110.438	111.7038	111.0386	110.9206	110.6178	111.1925	110.6904	110.7254	111.2375	110.7031	111.1445	110.6567	110.6887
D(2,1,4,3)	117.6672	114.7187	116.2531	116.5288	117.2409	115.8953	117.0696	116.9872	115.7908	117.0396	116.0068	117.1491	117.0736
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2439.53630874	-2439.7580617	-2439.80264523	-2439.80359299	-2441.92363764	-2441.95699103	-2441.96813101	-2441.96826246	-2441.95771924	-2441.96890634	-2441.96375896	-2441.97385144	-2441.97398034
ZPE Correction	0.035847	0.035539	0.035809	0.035599	0.035696	0.035318	0.035449	0.035386	0.035246	0.035409	0.03524	0.035412	0.035367

S2h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1063	1.1073	1.1044	1.1048	1.1022	1.1041	1.1019	1.1022	1.1032	1.101	1.1018	1.0996	1.0999
R(1,3)	1.1063	1.1073	1.1044	1.1048	1.1022	1.1041	1.1019	1.1022	1.1032	1.101	1.1018	1.0996	1.0999
R(1,4)	1.1063	1.1073	1.1044	1.1048	1.1022	1.1041	1.1019	1.1022	1.1032	1.101	1.1018	1.0996	1.0999
R(1,5)	2.0238	1.9864	1.9884	1.9886	2.0239	1.9995	2.0038	2.003	1.9917	1.9958	1.9927	1.9952	1.9943
A(2,1,3)	108.4768	107.1619	108.0158	108.1577	108.3884	107.8501	108.3898	108.3636	107.8112	108.3921	107.9364	108.4685	108.4375
A(2,1,4)	108.4768	107.1619	108.0158	108.1577	108.3884	107.8501	108.3898	108.3636	107.8112	108.3921	107.9364	108.4685	108.4375
A(2,1,5)	110.4482	111.6921	110.8902	110.7548	110.5335	111.0474	110.5322	110.5573	111.0842	110.5299	110.9656	110.4563	110.4862
A(3,1,4)	108.4768	107.1619	108.0158	108.1577	108.3884	107.8501	108.3898	108.3636	107.8112	108.3921	107.9364	108.4685	108.4375
A(3,1,5)	110.4482	111.6921	110.8902	110.7548	110.5335	111.0474	110.5322	110.5573	111.0842	110.5299	110.9656	110.4563	110.4862
A(4,1,5)	110.4482	111.6921	110.8902	110.7548	110.5335	111.0474	110.5322	110.5573	111.0842	110.5299	110.9656	110.4563	110.4862
D(2,1,4,3)	117.6428	114.7454	116.6002	116.918	117.4406	116.2328	117.4437	117.3841	116.1469	117.449	116.4237	117.6237	117.5527
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2438.62191705	-2438.84866259	-2438.89391499	-2438.89495481	-2441.00968583	-2441.04350036	-2441.05397394	-2441.05409813	-2441.04446547	-2441.05499115	-2441.05043816	-2441.0599727	-2441.0601052
ZPE Correction	0.034909	0.034585	0.034895	0.034696	0.034782	0.034393	0.034555	0.034503	0.034356	0.034544	0.034373	0.03456	0.03452

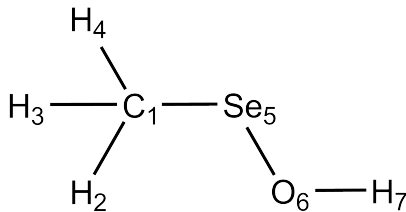
S2i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1006	1.1014	1.0989	1.0992	1.0963	1.0981	1.0964	1.0966	1.097	1.0953	1.0953	1.0936	1.0938
R(1,3)	1.1006	1.1014	1.0989	1.0992	1.0963	1.0981	1.0964	1.0966	1.097	1.0953	1.0953	1.0936	1.0938
R(1,4)	1.1006	1.1014	1.0989	1.0992	1.0963	1.0981	1.0964	1.0966	1.097	1.0953	1.0953	1.0936	1.0938
R(1,5)	2.0182	1.9812	1.9813	1.9817	2.0156	1.9922	1.9951	1.9946	1.9852	1.9878	1.9861	1.9876	1.987
A(2,1,3)	108.5578	107.3408	108.019	108.1714	108.455	107.989	108.3999	108.3866	107.9384	108.378	108.0607	108.4603	108.4421
A(2,1,4)	108.5578	107.3408	108.019	108.1714	108.455	107.989	108.3999	108.3866	107.9384	108.378	108.0607	108.4603	108.4421
A(2,1,5)	110.3699	111.5258	110.887	110.7417	110.4693	110.9157	110.5224	110.5352	110.9637	110.5435	110.8474	110.4641	110.4818
A(3,1,4)	108.5578	107.3408	108.019	108.1714	108.455	107.989	108.3999	108.3866	107.9384	108.378	108.0607	108.4603	108.4421
A(3,1,5)	110.3699	111.5258	110.887	110.7417	110.4693	110.9157	110.5224	110.5352	110.9637	110.5435	110.8474	110.4641	110.4818
A(4,1,5)	110.3699	111.5258	110.887	110.7417	110.4693	110.9157	110.5224	110.5352	110.9637	110.5435	110.8474	110.4641	110.4818
D(2,1,4,3)	117.8292	115.1261	116.6075	116.9488	117.5928	116.5405	117.4668	117.4365	116.4282	117.4168	116.7004	117.605	117.5632
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-2439.22252585	-2439.44657171	-2439.48777081	-2439.48880576	-2441.61066986	-2441.64297797	-2441.65109812	-2441.65120476	-2441.64424361	-2441.65238516	-2441.65011671	-2441.65753452	-2441.65764242
ZPE Correction	0.035618	0.035331	0.03562	0.035445	0.035492	0.035156	0.035287	0.035253	0.035141	0.035293	0.03516	0.035311	0.035285

S2j – QCISD

	QCISD/cc-pvtz
R(1,2)	1.0927
R(1,3)	1.0927
R(1,4)	1.0927
R(1,5)	1.9769
A(2,1,3)	107.7843
A(2,1,4)	107.7843
A(2,1,5)	111.1097
A(3,1,4)	107.7843
A(3,1,5)	111.1097
A(4,1,5)	111.1097
D(2,1,4,3)	116.0878
D(2,1,5,3)	-120.0000
D(2,1,5,4)	120.0000
D(3,1,5,4)	-120.0000
Energy	-2439.9581828
ZPE Correction	0.035874

S3 – MeSeOH



S3a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0893	1.0903	1.0911	1.0909	1.0858	1.0888	1.0886	1.0886	1.088	1.0877	1.0861	1.086	1.086
R(1,3)	1.089	1.0899	1.091	1.0908	1.0854	1.0884	1.0884	1.0884	1.0876	1.0876	1.086	1.0859	1.0859
R(1,4)	1.0927	1.0935	1.0949	1.0951	1.0896	1.0924	1.0927	1.0927	1.0914	1.0916	1.0897	1.0899	1.0899
R(1,5)	1.9871	1.957	1.953	1.9547	1.9791	1.961	1.9604	1.9604	1.9547	1.9538	1.9537	1.9534	1.9534
R(5,6)	1.9029	1.8327	1.8316	1.83	1.8878	1.8484	1.8527	1.8526	1.8192	1.8242	1.8224	1.8252	1.8251
R(6,7)	0.9825	0.968	0.9683	0.9686	0.9774	0.9643	0.9646	0.9646	0.9641	0.9645	0.9623	0.9629	0.9629
A(2,1,3)	111.455	111.2074	110.8187	111.1454	110.7546	111.0035	111.2348	111.2236	110.9732	111.1402	111.0786	111.1911	111.1901
A(2,1,4)	110.3341	109.6647	109.5485	109.5803	109.8769	109.7381	109.7247	109.7491	109.5975	109.628	109.7121	109.6933	109.6927
A(2,1,5)	110.1056	110.7679	111.2193	111.3742	110.7672	110.7784	110.9262	110.9405	110.9357	110.99	110.8946	110.7928	110.7821
A(3,1,4)	110.2138	109.6876	109.5839	109.6299	109.7798	109.7494	109.7119	109.7169	109.6628	109.6525	109.6914	109.71	109.7156
A(3,1,5)	107.6341	109.0998	109.5682	109.8873	108.3715	109.1278	109.2367	109.1737	109.5049	109.4418	109.2355	109.4319	109.438
A(4,1,5)	106.962	106.2885	105.9805	105.0409	107.2118	106.3309	105.8618	105.8941	106.0432	105.8473	106.1023	105.8814	105.8823
A(1,5,6)	95.5602	97.9315	98.3802	98.8627	96.6282	97.7391	97.9169	97.8993	98.4574	98.319	98.0708	98.2333	98.2347
A(5,6,7)	105.8793	104.8312	107.2114	107.2168	109.0866	105.408	106.4131	106.43	106.3644	107.188	107.0678	107.0881	107.0919
D(2,1,5,6)	-68.67	-66.5018	-67.0561	-66.7366	-69.2082	-66.5897	-66.9135	-67.2579	-66.1088	-66.7632	-67.5561	-66.1652	-66.0938
D(3,1,5,6)	53.0031	56.2321	55.8075	56.8726	52.4788	55.9142	56.0521	55.6601	56.7164	56.2659	55.1911	56.7897	56.8567
D(4,1,5,6)	171.4277	174.436	173.9604	174.7206	170.9146	174.2287	174.1207	173.7202	174.9647	174.3611	173.3669	174.9663	175.0436
D(1,5,6,7)	95.1426	92.4095	94.0488	94.0428	94.1449	92.4363	94.2524	94.1716	91.9266	93.6007	93.4492	93.5395	93.5463
Energy	-2514.8336366	-2515.09603069	-2515.12708155	-2515.12836591	-2517.23847204	-2517.2991727	-2517.30571021	-2517.3058338	-2517.31006076	-2517.31520147	-2517.31975674	-2517.32273177	-2517.32278635
ZPE Correction	0.050788	0.050976	0.05078	0.050725	0.050597	0.050553	0.050451	0.050452	0.050614	0.050555	0.050662	0.05063	0.050625

S3b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0889	1.09	1.0907	1.0905	1.0859	1.0889	1.0887	1.0887	1.0882	1.088	1.0865	1.0864	1.0864
R(1,3)	1.0888	1.0897	1.0906	1.0904	1.0857	1.0886	1.0886	1.0886	1.088	1.0879	1.0865	1.0863	1.0863
R(1,4)	1.0923	1.0932	1.0943	1.0946	1.0899	1.0925	1.0928	1.0927	1.0916	1.0918	1.0901	1.0902	1.0902
R(1,5)	1.9675	1.938	1.9339	1.9353	1.9591	1.9421	1.9414	1.9415	1.9363	1.9354	1.9353	1.935	1.935
R(5,6)	1.8879	1.8176	1.8153	1.8138	1.8726	1.833	1.836	1.836	1.8047	1.8082	1.8075	1.8093	1.8093
R(6,7)	0.98	0.9657	0.9662	0.9664	0.975	0.9625	0.9629	0.9629	0.9625	0.9629	0.961	0.9614	0.9614
A(2,1,3)	111.3597	111.1917	110.7448	111.059	110.6362	110.991	111.1838	111.1739	110.9692	111.1101	111.0626	111.1562	111.1563
A(2,1,4)	110.1744	109.509	109.3709	109.3852	109.6539	109.568	109.5392	109.5664	109.4481	109.4653	109.551	109.5219	109.5206
A(2,1,5)	110.4026	111.0677	111.5148	111.6844	111.1053	111.1001	111.2267	111.2383	111.233	111.2777	111.1666	111.0847	111.0746
A(3,1,4)	109.9643	109.4586	109.3488	109.3926	109.4743	109.5114	109.473	109.4788	109.4487	109.4342	109.4732	109.4874	109.4931
A(3,1,5)	107.7391	109.2079	109.6961	110.0566	108.6356	109.2882	109.3933	109.3282	109.6304	109.5754	109.3863	109.5733	109.5805
A(4,1,5)	107.0803	106.2759	106.0393	105.0743	107.2599	106.2622	105.8771	105.9094	105.9781	105.8304	106.0686	105.8723	105.8709
A(1,5,6)	95.6397	98.0326	98.4267	98.9293	96.682	97.8716	97.9963	97.9793	98.5421	98.3933	98.177	98.3197	98.3237
A(5,6,7)	106.1336	104.8191	107.0573	107.0634	109.2791	105.3333	106.2417	106.252	106.262	106.9972	106.8127	106.8783	106.8793
D(2,1,5,6)	-69.2909	-67.2153	-67.7613	-67.266	-69.602	-67.1536	-67.4415	-67.7419	-66.7812	-67.3134	-67.9461	-66.7232	-66.6439
D(3,1,5,6)	52.5108	55.7703	55.2983	56.571	52.325	55.6554	55.7686	55.4182	56.3259	55.9646	55.0651	56.4808	56.5584
D(4,1,5,6)	170.7602	173.7532	173.2725	174.2428	170.567	173.7345	173.6444	173.2855	174.35	173.8617	173.043	174.4626	174.5499
D(1,5,6,7)	95.2635	92.4784	93.8476	93.8276	94.2796	92.4791	93.9644	93.902	92.0683	93.4097	93.1881	93.2499	93.2518
Energy	-2515.93541087	-2516.19880706	-2516.2273659	-2516.22858153	-2518.34065331	-2518.40271361	-2518.40805836	-2518.40819987	-2518.41400559	-2518.41809666	-2518.42321989	-2518.4255617	-2518.42561522
ZPE Correction	0.051162	0.051282	0.051106	0.051053	0.050939	0.050831	0.05073	0.050735	0.050874	0.050821	0.050902	0.050876	0.050871

S3c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0895	1.0906	1.0914	1.0912	1.0867	1.0896	1.0895	1.0895	1.089	1.0888	1.0874	1.0873	1.0873
R(1,3)	1.0894	1.0903	1.0913	1.0911	1.0864	1.0893	1.0893	1.0894	1.0887	1.0887	1.0873	1.0872	1.0872
R(1,4)	1.0929	1.0938	1.095	1.0952	1.0906	1.0932	1.0935	1.0934	1.0924	1.0926	1.091	1.0911	1.0911
R(1,5)	1.9711	1.9413	1.9371	1.9386	1.9629	1.9455	1.9449	1.9449	1.9398	1.9389	1.9388	1.9385	1.9385
R(5,6)	1.8913	1.8204	1.8181	1.8166	1.8764	1.8364	1.8395	1.8394	1.8078	1.8113	1.8106	1.8125	1.8125
R(6,7)	0.9803	0.9659	0.9663	0.9665	0.9752	0.9627	0.963	0.963	0.9626	0.963	0.9612	0.9615	0.9615
A(2,1,3)	111.3767	111.1887	110.7425	111.055	110.6562	110.9931	111.184	111.173	110.9722	111.1128	111.0571	111.1546	111.1543
A(2,1,4)	110.183	109.5075	109.3657	109.3872	109.664	109.5668	109.5388	109.5658	109.4495	109.4663	109.5467	109.5186	109.5174
A(2,1,5)	110.3713	111.047	111.5022	111.6672	111.0736	111.08	111.2164	111.2276	111.2106	111.266	111.1629	111.0824	111.0707
A(3,1,4)	109.9853	109.4702	109.3549	109.4026	109.5029	109.527	109.4852	109.4909	109.4651	109.4466	109.4802	109.494	109.5007
A(3,1,5)	107.779	109.2463	109.7457	110.0903	108.6844	109.3392	109.4417	109.3787	109.6748	109.6178	109.4318	109.6183	109.6258
A(4,1,5)	107.0226	106.2508	106.0024	105.0493	107.1824	106.2134	105.825	105.8572	105.9338	105.7818	106.0284	105.8261	105.8252
A(1,5,6)	95.7344	98.1213	98.5407	99.0309	96.8017	97.9676	98.1062	98.09	98.631	98.4951	98.2735	98.429	98.4325
A(5,6,7)	106.0141	104.7798	107.0028	107.0047	109.1197	105.2355	106.1413	106.1532	106.1629	106.8989	106.7077	106.7747	106.7764
D(2,1,5,6)	-69.1036	-67.0527	-67.5772	-67.1349	-69.3831	-66.9448	-67.287	-67.5928	-66.5673	-67.1706	-67.8113	-66.598	-66.5122
D(3,1,5,6)	52.7255	55.9416	55.5058	56.7092	52.581	55.8884	55.9501	55.594	56.5592	56.1325	55.2219	56.6336	56.7164
D(4,1,5,6)	170.9898	173.9442	173.4922	174.3955	170.8402	173.9853	173.8362	173.4726	174.6009	174.0388	173.2091	174.6206	174.7146
D(1,5,6,7)	95.2058	92.4236	93.7967	93.7859	94.2211	92.4431	93.9031	93.8302	92.0131	93.3545	93.1648	93.2125	93.2127
Energy	-2514.76953889	-2515.03293728	-2515.06165293	-2515.06287912	-2517.17160775	-2517.2336945	-2517.23916772	-2517.2393205	-2517.24476879	-2517.24899518	-2517.25400448	-2517.25648382	-2517.25654376
ZPE Correction	0.051102	0.051228	0.051057	0.051003	0.05087	0.050771	0.050673	0.050676	0.050809	0.050758	0.050835	0.050808	0.050803

S3d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0965	1.0971	1.0978	1.0977	1.0934	1.0958	1.0956	1.0956	1.095	1.0948	1.0934	1.0932	1.0933
R(1,3)	1.0959	1.0964	1.0975	1.0973	1.0927	1.0952	1.0952	1.0953	1.0945	1.0945	1.0931	1.093	1.093
R(1,4)	1.0998	1.1001	1.1014	1.1016	1.0972	1.0992	1.0995	1.0995	1.0982	1.0985	1.0968	1.097	1.097
R(1,5)	2.0125	1.9763	1.971	1.973	2.0018	1.9801	1.9791	1.9791	1.9737	1.9725	1.9717	1.9712	1.9712
R(5,6)	1.9233	1.8463	1.8452	1.8435	1.9077	1.8631	1.8677	1.8676	1.8333	1.8385	1.8362	1.8392	1.8392
R(6,7)	0.9899	0.9723	0.9726	0.9729	0.9843	0.9687	0.969	0.969	0.9685	0.9688	0.9669	0.9673	0.9673
A(2,1,3)	111.6529	111.2788	110.8827	111.2318	110.8908	111.0688	111.3083	111.2934	111.065	111.238	111.1468	111.2672	111.266
A(2,1,4)	110.5737	109.7916	109.6507	109.6951	110.0344	109.8366	109.8261	109.8529	109.7209	109.7557	109.8251	109.7987	109.798
A(2,1,5)	109.797	110.5783	111.0855	111.2287	110.5723	110.59	110.7892	110.8048	110.7216	110.8161	110.7528	110.635	110.6205
A(3,1,4)	110.4628	109.8415	109.7042	109.7696	109.9436	109.8749	109.8262	109.8318	109.8141	109.7954	109.8115	109.835	109.8426
A(3,1,5)	107.2196	108.9334	109.456	109.7679	108.244	109.0249	109.1049	109.0363	109.3915	109.2884	109.0986	109.3201	109.3287
A(4,1,5)	106.9677	106.2896	105.9385	104.9606	107.0648	106.3308	105.8376	105.875	106.0009	105.8015	106.0763	105.8403	105.8407
A(1,5,6)	95.5352	98.1099	98.6021	99.0691	96.828	97.931	98.1096	98.0894	98.6245	98.4883	98.262	98.4229	98.4247
A(5,6,7)	104.2048	103.7324	106.1178	106.1302	107.4832	104.21	105.2133	105.2307	105.1371	105.9639	105.8221	105.861	105.8663
D(2,1,5,6)	-68.871	-66.3431	-66.9082	-66.4731	-68.9753	-66.1877	-66.7868	-67.1682	-65.6883	-66.6046	-67.5128	-65.8957	-65.8024
D(3,1,5,6)	52.6039	56.2453	55.8693	57.0613	52.6764	56.2067	56.0911	55.6549	57.0331	56.3271	55.1344	56.9743	57.0623
D(4,1,5,6)	171.1083	174.5449	174.0832	174.9699	171.158	174.6156	174.2138	173.7698	175.3778	174.4871	173.367	175.2183	175.3199
D(1,5,6,7)	93.7125	91.301	92.7041	92.759	92.8934	91.3197	92.9321	92.8361	90.8411	92.3361	92.2162	92.2594	92.2577
Energy	-2515.97416714	-2516.22826214	-2516.2585898	-2516.25987456	-2518.36205595	-2518.4209427	-2518.42731151	-2518.42745031	-2518.43116993	-2518.43617083	-2518.43980856	-2518.44274764	-2518.44281222
ZPE Correction	0.049274	0.04951	0.049324	0.049265	0.049053	0.049113	0.049002	0.049001	0.049151	0.049091	0.04918	0.049151	0.049144

S3e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0912	1.0921	1.0929	1.0927	1.0879	1.0908	1.0907	1.0907	1.0902	1.09	1.0885	1.0884	1.0884
R(1,3)	1.091	1.0918	1.0928	1.0926	1.0877	1.0905	1.0906	1.0906	1.0899	1.0899	1.0885	1.0883	1.0883
R(1,4)	1.0945	1.0953	1.0966	1.0968	1.0918	1.0944	1.0947	1.0947	1.0936	1.0938	1.0921	1.0923	1.0923
R(1,5)	1.9816	1.9524	1.9482	1.9499	1.9727	1.956	1.9554	1.9555	1.9505	1.9496	1.9494	1.9492	1.9492
R(5,6)	1.8975	1.8255	1.8237	1.8222	1.8822	1.8417	1.8455	1.8454	1.8126	1.8169	1.8158	1.8182	1.8182
R(6,7)	0.9808	0.9667	0.967	0.9672	0.9755	0.9632	0.9635	0.9636	0.9631	0.9635	0.9616	0.9621	0.9621
A(2,1,3)	111.4496	111.2257	110.8031	111.1266	110.7153	111.0189	111.2332	111.2196	111.0079	111.1633	111.0923	111.1956	111.1951
A(2,1,4)	110.3104	109.6444	109.5071	109.5334	109.7928	109.6887	109.6716	109.6979	109.5706	109.5977	109.6737	109.6505	109.6494
A(2,1,5)	110.1779	110.8327	111.2955	111.4524	110.8885	110.8757	111.0113	111.0247	111.0028	111.0575	110.9649	110.8726	110.8629
A(3,1,4)	110.1516	109.6373	109.5177	109.5664	109.6663	109.6784	109.6392	109.6459	109.6147	109.6012	109.6304	109.6472	109.6526
A(3,1,5)	107.6027	109.0612	109.5446	109.8782	108.483	109.147	109.245	109.1786	109.5015	109.4312	109.2357	109.4334	109.4396
A(4,1,5)	107.0151	106.3137	106.0522	105.1025	107.2175	106.3171	105.8957	105.9315	106.0156	105.8462	106.1161	105.9006	105.9004
A(1,5,6)	95.5093	97.9262	98.3589	98.8503	96.5839	97.7453	97.8966	97.8773	98.4635	98.3182	98.071	98.226	98.2286
A(5,6,7)	105.8183	104.6817	106.9517	106.9565	108.9177	105.1442	106.0859	106.1024	106.0614	106.8336	106.6795	106.7291	106.7333
D(2,1,5,6)	-69.1274	-66.9297	-67.5382	-67.093	-69.4999	-66.8941	-67.2276	-67.5835	-66.4073	-67.0357	-67.8076	-66.4369	-66.3719
D(3,1,5,6)	52.5627	55.8436	55.3407	56.54	52.2873	55.7057	55.7983	55.3886	56.5042	56.0607	55.0034	56.5779	56.64
D(4,1,5,6)	170.9262	173.982	173.4433	174.343	170.6516	173.9388	173.8043	173.3883	174.6787	174.0896	173.1152	174.6919	174.7635
D(1,5,6,7)	95.1461	92.2935	93.7322	93.7081	94.1532	92.2333	93.8797	93.7904	91.7716	93.2723	93.0556	93.1639	93.1695
Energy	-2514.62229112	-2514.88422028	-2514.91375319	-2514.91500176	-2517.02859028	-2517.09016357	-2517.09614832	-2517.09627879	-2517.10123073	-2517.10588566	-2517.11046903	-2517.11318424	-2517.11323845
ZPE Correction	0.050913	0.051058	0.050887	0.050831	0.050734	0.050634	0.050534	0.050539	0.050682	0.050627	0.050705	0.050671	0.050666

S3f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0904	1.0914	1.0922	1.0921	1.0871	1.0902	1.0901	1.0902	1.0898	1.0897	1.0888	1.0886	1.0886
R(1,3)	1.09	1.0909	1.092	1.0918	1.0866	1.0898	1.0899	1.0899	1.0894	1.0895	1.0886	1.0885	1.0885
R(1,4)	1.0938	1.0944	1.0958	1.096	1.0912	1.0939	1.0943	1.0942	1.0931	1.0936	1.0923	1.0925	1.0925
R(1,5)	1.979	1.9434	1.9391	1.9406	1.9703	1.9498	1.949	1.9489	1.9444	1.9434	1.9424	1.9421	1.942
R(5,6)	1.9106	1.8324	1.8318	1.8301	1.8948	1.8497	1.8552	1.8551	1.8182	1.8241	1.822	1.8255	1.8254
R(6,7)	0.9835	0.9663	0.9665	0.9668	0.9773	0.9631	0.9633	0.9633	0.963	0.9633	0.9613	0.9619	0.9619
A(2,1,3)	111.4347	111.091	110.6747	111.0014	110.6886	110.935	111.2063	111.1833	110.9323	111.1267	110.992	111.113	111.1154
A(2,1,4)	110.1614	109.3662	109.2218	109.2508	109.6538	109.4856	109.4681	109.4921	109.3606	109.3994	109.4592	109.4416	109.4391
A(2,1,5)	110.3714	111.1718	111.6712	111.8668	111.0686	111.1049	111.294	111.3176	111.2784	111.3557	111.313	111.2105	111.2065
A(3,1,4)	109.9979	109.3717	109.2393	109.2771	109.5258	109.4951	109.4352	109.4379	109.4138	109.3935	109.3973	109.4173	109.4204
A(3,1,5)	108.0117	109.6177	110.1289	110.4389	108.9713	109.6651	109.7396	109.6746	109.9913	109.9	109.7202	109.9058	109.91
A(4,1,5)	106.7316	106.0859	105.7617	104.7951	106.8461	106.0278	105.5304	105.5715	105.7187	105.4985	105.8155	105.5933	105.59
A(1,5,6)	96.2774	98.5741	99.0665	99.5459	97.5551	98.4783	98.654	98.6338	99.18	99.0524	98.7538	98.9027	98.9054
A(5,6,7)	104.265	103.7252	106.0808	106.1226	107.5036	104.1757	105.1552	105.1862	105.1487	105.9594	105.9005	105.8952	105.9086
D(2,1,5,6)	-68.0457	-66.2297	-66.8793	-66.8595	-68.2381	-65.9029	-66.4817	-66.9309	-65.8312	-66.6339	-67.5461	-66.1274	-66.1217
D(3,1,5,6)	54.0034	56.9815	56.5063	57.3126	53.9551	57.098	57.0452	56.5371	57.5129	56.9476	55.7072	57.3401	57.3491
D(4,1,5,6)	172.2488	174.9682	174.4181	174.8823	172.2082	175.2227	174.8608	174.3459	175.5361	174.7773	173.6264	175.2537	175.2666
D(1,5,6,7)	94.491	92.1488	93.6427	93.5261	93.8314	92.2352	94.0722	93.9354	91.7409	93.4538	93.3362	93.536	93.5557
Energy	-2516.11187624	-2516.36940368	-2516.4005141	-2516.40185245	-2518.49782313	-2518.55942115	-2518.56654982	-2518.56667741	-2518.56992938	-2518.57555801	-2518.57888098	-2518.58223673	-2518.58231715
ZPE Correction	0.050403	0.050582	0.050397	0.050336	0.050261	0.050197	0.050084	0.050078	0.050196	0.050122	0.050187	0.050152	0.050147

S3g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0897	1.0907	1.0915	1.0914	1.0866	1.0897	1.0896	1.0897	1.0892	1.0891	1.0881	1.0879	1.088
R(1,3)	1.0893	1.0902	1.0913	1.0912	1.0861	1.0893	1.0894	1.0894	1.0888	1.0889	1.0879	1.0878	1.0878
R(1,4)	1.0929	1.0937	1.095	1.0953	1.0904	1.0932	1.0936	1.0936	1.0925	1.0929	1.0916	1.0917	1.0917
R(1,5)	1.977	1.9446	1.9403	1.9418	1.9682	1.9496	1.949	1.949	1.9443	1.9435	1.9428	1.9426	1.9425
R(5,6)	1.9001	1.825	1.8235	1.8219	1.8844	1.8416	1.8462	1.8461	1.8115	1.8165	1.8148	1.8178	1.8178
R(6,7)	0.9813	0.9658	0.9659	0.9662	0.9753	0.9624	0.9626	0.9627	0.9624	0.9626	0.9607	0.9613	0.9613
A(2,1,3)	111.4066	111.1184	110.7008	111.0076	110.6686	110.94	111.1818	111.1589	110.9332	111.1132	110.9853	111.1103	111.1094
A(2,1,4)	110.1768	109.4437	109.2985	109.3312	109.6618	109.5294	109.5098	109.5361	109.4092	109.4451	109.5029	109.4813	109.4801
A(2,1,5)	110.3208	111.0659	111.5599	111.7336	111.0264	111.0589	111.2411	111.2564	111.201	111.2895	111.2388	111.145	111.1352
A(3,1,4)	110.0276	109.4468	109.3148	109.3637	109.5571	109.539	109.4814	109.4866	109.4689	109.4444	109.4479	109.4671	109.4732
A(3,1,5)	107.9436	109.4511	109.9737	110.289	108.8841	109.533	109.6345	109.5726	109.8687	109.7911	109.5981	109.8037	109.8093
A(4,1,5)	106.8372	106.1845	105.8584	104.9185	106.961	106.1185	105.6334	105.6747	105.8217	105.5987	105.932	105.6807	105.6813
A(1,5,6)	96.052	98.3897	98.9176	99.3877	97.2625	98.2752	98.4928	98.4707	98.9697	98.884	98.5784	98.7798	98.7802
A(5,6,7)	105.167	104.3203	106.5818	106.6087	108.2801	104.6767	105.6297	105.6574	105.5993	106.3939	106.2833	106.2958	106.3068
D(2,1,5,6)	-68.3311	-66.5429	-67.1454	-66.9489	-68.5597	-66.3187	-66.8217	-67.2144	-66.0328	-66.8496	-67.7245	-66.3143	-66.2708
D(3,1,5,6)	53.6088	56.516	56.0853	57.0256	53.5227	56.5662	56.5639	56.1091	57.173	56.5918	55.3844	57.0331	57.0725
D(4,1,5,6)	171.9099	174.5602	174.061	174.692	171.8301	174.7249	174.4377	173.9806	175.2561	174.4821	173.3655	175.0021	175.0519
D(1,5,6,7)	94.7762	92.1213	93.5923	93.5256	93.9132	92.151	93.8516	93.7266	91.6217	93.2342	93.1616	93.2472	93.2584
Energy	-2515.27051753	-2515.53074894	-2515.56151772	-2515.56283266	-2517.66861913	-2517.73109318	-2517.73805414	-2517.73820898	-2517.74183034	-2517.74739384	-2517.75103444	-2517.7544945	-2517.75457867
ZPE Correction	0.05089	0.051054	0.050885	0.050819	0.050736	0.050632	0.05053	0.050525	0.050646	0.050587	0.05065	0.050612	0.050605

S3h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0976	1.0983	1.0992	1.099	1.0945	1.0969	1.0967	1.0967	1.0963	1.0961	1.0947	1.0946	1.0946
R(1,3)	1.0974	1.0979	1.0991	1.0989	1.0942	1.0966	1.0967	1.0967	1.096	1.096	1.0947	1.0946	1.0946
R(1,4)	1.1013	1.1016	1.1031	1.1034	1.0986	1.1008	1.1012	1.1011	1.0999	1.1003	1.0986	1.0988	1.0988
R(1,5)	1.9881	1.9568	1.9518	1.9535	1.9804	1.9615	1.9603	1.9603	1.9554	1.954	1.9538	1.9533	1.9533
R(5,6)	1.9189	1.844	1.8437	1.8421	1.9053	1.8615	1.8668	1.8667	1.8319	1.8375	1.8355	1.8388	1.8387
R(6,7)	0.9941	0.977	0.9772	0.9775	0.9888	0.9737	0.9738	0.9739	0.9734	0.9738	0.9717	0.9723	0.9723
A(2,1,3)	111.5486	111.3239	110.8989	111.2497	110.7871	111.1122	111.3699	111.3555	111.1407	111.323	111.2298	111.3573	111.3553
A(2,1,4)	110.2598	109.5546	109.4038	109.4224	109.7693	109.6244	109.6104	109.6402	109.5259	109.5589	109.6437	109.6038	109.6022
A(2,1,5)	110.347	111.0195	111.5269	111.6988	111.0533	111.0114	111.2343	111.2497	111.1478	111.2276	111.1437	111.0279	111.0162
A(3,1,4)	110.0064	109.4952	109.3493	109.3978	109.5375	109.5638	109.4849	109.4895	109.516	109.4885	109.5166	109.541	109.5482
A(3,1,5)	107.6318	109.2027	109.7392	110.0966	108.5517	109.2663	109.3574	109.288	109.6167	109.525	109.3117	109.5547	109.5631
A(4,1,5)	106.9075	106.1018	105.778	104.7584	107.0546	106.1333	105.6138	105.6504	105.744	105.5472	105.8454	105.5887	105.5887
A(1,5,6)	95.7377	98.2135	98.6585	99.1733	96.9189	98.0255	98.194	98.1736	98.7439	98.5635	98.3063	98.4789	98.4808
A(5,6,7)	103.9125	103.268	105.7466	105.7701	107.1815	103.7619	104.7921	104.8129	104.6775	105.5435	105.4258	105.4303	105.4383
D(2,1,5,6)	-69.2274	-66.9197	-67.4782	-67.0335	-69.5498	-66.9284	-67.4878	-67.8561	-66.4096	-67.216	-68.1143	-66.4816	-66.4115
D(3,1,5,6)	52.7042	56.197	55.8167	57.0885	52.4764	55.9594	55.9385	55.5138	56.8476	56.2633	55.0416	56.9259	56.9915
D(4,1,5,6)	170.8565	174.1249	173.6681	174.6118	170.6363	174.0179	173.6663	173.2322	174.8142	174.0431	172.9098	174.8049	174.8832
D(1,5,6,7)	94.3893	92.1454	93.7735	93.7745	93.5325	92.0785	93.9463	93.8559	91.6793	93.366	93.1733	93.2865	93.2921
Energy	-2514.30834588	-2514.57110144	-2514.60253093	-2514.6038239	-2516.7058466	-2516.76707252	-2516.77404587	-2516.77417938	-2516.77749138	-2516.7829837	-2516.78691113	-2516.79010647	-2516.79017289
ZPE Correction	0.049484	0.049631	0.049435	0.049367	0.04926	0.049207	0.049093	0.04909	0.049234	0.049175	0.049266	0.049231	0.049224

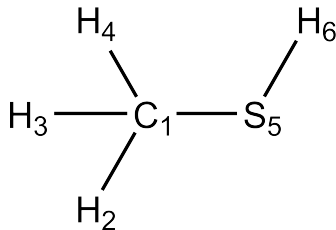
S3i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0917	1.0926	1.0933	1.0932	1.0884	1.0911	1.0909	1.0909	1.0904	1.0902	1.0886	1.0885	1.0885
R(1,3)	1.0915	1.0922	1.0932	1.093	1.0881	1.0907	1.0908	1.0908	1.0901	1.0901	1.0885	1.0883	1.0884
R(1,4)	1.0951	1.0958	1.0971	1.0973	1.0923	1.0947	1.095	1.095	1.0938	1.0941	1.0922	1.0924	1.0924
R(1,5)	1.9805	1.9503	1.946	1.9476	1.9709	1.9537	1.953	1.953	1.9481	1.9471	1.947	1.9466	1.9467
R(5,6)	1.899	1.8266	1.8246	1.823	1.8833	1.842	1.8454	1.8453	1.814	1.8179	1.8165	1.8187	1.8186
R(6,7)	0.9829	0.9676	0.968	0.9683	0.9775	0.9641	0.9644	0.9644	0.964	0.9643	0.9625	0.9628	0.9628
A(2,1,3)	111.4783	111.249	110.8158	111.1413	110.7589	111.0616	111.2632	111.2512	111.0488	111.1941	111.1255	111.2299	111.2293
A(2,1,4)	110.3121	109.6369	109.4977	109.5207	109.8018	109.693	109.6728	109.7002	109.5783	109.6026	109.6783	109.6521	109.6511
A(2,1,5)	110.2183	110.9057	111.3707	111.5283	110.9208	110.9221	111.0643	111.0756	111.0462	111.1024	111.0086	110.9232	110.9112
A(3,1,4)	110.1289	109.6062	109.4847	109.5354	109.6449	109.6599	109.6207	109.6269	109.6018	109.5862	109.6141	109.6307	109.6374
A(3,1,5)	107.6308	109.0947	109.5863	109.9316	108.524	109.18	109.2707	109.2059	109.5186	109.4461	109.2696	109.4579	109.4652
A(4,1,5)	106.9352	106.2163	105.959	104.9939	107.108	106.2022	105.7978	105.8317	105.9124	105.7596	106.0105	105.7989	105.7988
A(1,5,6)	95.6204	98.027	98.4449	98.9385	96.7249	97.8829	98.0186	98.0022	98.5544	98.4015	98.1901	98.342	98.3446
A(5,6,7)	105.4869	104.5168	106.8042	106.81	108.7065	105.0229	105.9517	105.9634	105.9472	106.7058	106.5142	106.5785	106.5806
D(2,1,5,6)	-69.0246	-67.0787	-67.6733	-67.1482	-69.3127	-66.893	-67.2807	-67.6062	-66.4858	-67.1362	-67.8147	-66.5402	-66.4555
D(3,1,5,6)	52.7425	55.7946	55.3017	56.5948	52.576	55.8133	55.836	55.4583	56.5183	56.0397	55.0902	56.5687	56.6495
D(4,1,5,6)	171.0521	173.8604	173.3351	174.328	170.877	173.9783	173.7797	173.395	174.6292	174.0108	173.1421	174.6198	174.7122
D(1,5,6,7)	95.1681	92.4441	93.8775	93.8669	94.301	92.5093	94.0513	93.974	92.0873	93.4885	93.2323	93.2904	93.2918
Energy	-2514.9590959	-2515.22025729	-2515.24946797	-2515.25071392	-2517.35813364	-2517.4187001	-2517.42434148	-2517.42448584	-2517.42957035	-2517.43393956	-2517.43879126	-2517.44134645	-2517.44140402
ZPE Correction	0.050638	0.050784	0.050616	0.050561	0.050428	0.050379	0.050281	0.050285	0.050423	0.050372	0.050474	0.050444	0.050438

S3j – QCISD

	QCISD/cc-pvtz
R(1,2)	1.0865
R(1,3)	1.0863
R(1,4)	1.09
R(1,5)	1.9333
R(5,6)	1.8013
R(6,7)	0.9596
A(2,1,3)	110.7589
A(2,1,4)	109.4453
A(2,1,5)	110.9242
A(3,1,4)	109.5239
A(3,1,5)	109.5335
A(4,1,5)	106.5582
A(1,5,6)	97.6657
A(5,6,7)	106.2833
D(2,1,5,6)	-65.8844
D(3,1,5,6)	56.6823
D(4,1,5,6)	175.0698
D(1,5,6,7)	92.0454
Energy	-2515.6374965
ZPE Correction	0.051119

S4 – MeSH



S4a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0902	1.0911	1.0917	1.0917	1.085	1.0892	1.0895	1.0893	1.0881	1.0883	1.0865	1.0866	1.0866
R(1,3)	1.0903	1.0911	1.0917	1.0917	1.0851	1.0892	1.0895	1.0893	1.0881	1.0883	1.0865	1.0866	1.0866
R(1,4)	1.0902	1.0913	1.0918	1.0918	1.0852	1.0897	1.0898	1.0897	1.0889	1.089	1.0874	1.0874	1.0875
R(1,5)	1.8985	1.8362	1.8366	1.8369	1.9022	1.8357	1.8353	1.8356	1.8281	1.8275	1.8239	1.8241	1.8242
R(5,6)	1.3801	1.3485	1.3486	1.3487	1.3849	1.3487	1.3485	1.3484	1.345	1.3448	1.3423	1.3422	1.3423
A(2,1,3)	110.9785	110.277	110.2087	110.2419	111.1088	110.4076	110.3457	110.3708	110.4332	110.3824	110.3731	110.388	110.383
A(2,1,4)	109.7067	108.7623	108.7131	108.73	109.7246	108.786	108.7919	108.8355	108.8179	108.8161	108.7996	108.8123	108.8088
A(2,1,5)	110.3705	111.396	111.4406	111.4114	110.3514	111.3203	111.3251	111.3204	111.2874	111.3012	111.2917	111.2765	111.2825
A(3,1,4)	109.7057	108.7599	108.7063	108.7177	109.7235	108.7899	108.7918	108.8096	108.8223	108.8255	108.8047	108.8173	108.8138
A(3,1,5)	110.4106	111.3551	111.416	111.4011	110.396	111.3251	111.3248	111.2456	111.2904	111.3036	111.2951	111.2798	111.2861
A(4,1,5)	105.526	106.1418	106.2071	106.1894	105.38	106.0582	106.1127	106.1126	106.0371	106.0623	106.1292	106.1197	106.1193
A(1,5,6)	96.8755	97.0003	97.0199	97.0221	96.6732	96.9671	96.9392	96.9359	97.1606	97.1462	97.2824	97.2691	97.2795
D(2,1,5,6)	-61.56	-61.7292	-61.6457	-61.7789	-61.6561	-61.7526	-61.7268	-61.6733	-61.813	-61.6785	-61.7772	-61.7761	-61.777
D(3,1,5,6)	61.5093	61.8334	61.9052	61.783	61.5552	61.9024	61.8512	61.8762	61.8261	61.9143	61.7904	61.7888	61.7902
D(4,1,5,6)	179.9845	180.0396	180.119	179.9919	179.9604	180.0785	180.0621	180.0659	180.01	180.1242	180.0105	180.0102	180.0106
Energy	-438.660877581	-438.705661503	-438.708420525	-438.708519151	-438.699598078	-438.742623058	-438.743219526	-438.743497448	-438.748907083	-438.749566078	-438.7532807	-438.753540652	-438.753622571
ZPE Correction	0.046003	0.046236	0.046103	0.046082	0.045534	0.045931	0.045872	0.04589	0.045848	0.045812	0.045911	0.045895	0.045889

S4b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0897	1.0909	1.0913	1.0913	1.0853	1.0894	1.0896	1.0895	1.0884	1.0885	1.0869	1.0869	1.0869
R(1,3)	1.0897	1.0909	1.0913	1.0913	1.0853	1.0894	1.0896	1.0895	1.0884	1.0885	1.0869	1.0869	1.0869
R(1,4)	1.0897	1.091	1.0913	1.0913	1.0855	1.0897	1.0898	1.0897	1.0891	1.0892	1.0877	1.0877	1.0877
R(1,5)	1.882	1.821	1.8214	1.8213	1.8833	1.8201	1.8198	1.8201	1.8125	1.8124	1.8087	1.8091	1.8091
R(5,6)	1.3762	1.3454	1.3455	1.3456	1.3818	1.3464	1.3463	1.3462	1.3429	1.3428	1.3407	1.3406	1.3407
A(2,1,3)	110.8509	110.1927	110.1427	110.1439	110.9378	110.3273	110.2687	110.2934	110.3615	110.3448	110.3121	110.3389	110.3306
A(2,1,4)	109.4863	108.5396	108.5122	108.5205	109.4543	108.5768	108.5905	108.6302	108.6345	108.6452	108.6107	108.6361	108.6326
A(2,1,5)	110.6107	111.582	111.6091	111.5956	110.6493	111.5388	111.5263	111.5084	111.5005	111.4664	111.4908	111.4663	111.4752
A(3,1,4)	109.4726	108.5447	108.5175	108.5259	109.4448	108.5766	108.5869	108.6024	108.6432	108.6536	108.631	108.6442	108.6419
A(3,1,5)	110.5948	111.5826	111.6094	111.5956	110.6368	111.5233	111.5186	111.459	111.4663	111.4665	111.4754	111.449	111.4542
A(4,1,5)	105.6881	106.2326	106.284	106.2949	105.5689	106.1266	106.1845	106.1848	106.0665	106.0995	106.1568	106.1431	106.1428
A(1,5,6)	96.9554	96.9825	96.9737	96.9767	96.719	96.9205	96.9088	96.8915	97.106	97.0954	97.2308	97.2173	97.2282
D(2,1,5,6)	-61.6215	-61.8726	-61.8601	-61.8497	-61.6697	-61.9215	-61.8506	-61.8902	-61.7847	-61.8893	-61.7437	-61.7784	-61.7691
D(3,1,5,6)	61.5785	61.884	61.8711	61.8629	61.6973	61.935	61.9168	61.8522	62.046	61.8947	62.0221	61.9849	61.9939
D(4,1,5,6)	179.9662	-179.9911	-179.9912	-179.9902	-179.9952	-179.9975	-179.9711	179.9509	-179.8733	-179.9922	-179.8527	-179.8965	-179.8876
Energy	-439.145827734	-439.190774049	-439.192504431	-439.192609846	-439.18206111	-439.225533299	-439.226270371	-439.226598682	-439.232108022	-439.232905782	-439.236308601	-439.23662949	-439.236723744
ZPE Correction	0.046296	0.046461	0.046354	0.046339	0.045848	0.046152	0.046096	0.04612	0.046047	0.046016	0.046092	0.046077	0.046071

S4c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0904	1.0916	1.092	1.0919	1.086	1.0901	1.0903	1.0903	1.0891	1.0893	1.0878	1.0878	1.0878
R(1,3)	1.0905	1.0916	1.092	1.092	1.086	1.0901	1.0903	1.0902	1.0891	1.0893	1.0878	1.0878	1.0878
R(1,4)	1.0904	1.0917	1.092	1.0919	1.0861	1.0904	1.0906	1.0905	1.0899	1.09	1.0885	1.0886	1.0886
R(1,5)	1.8844	1.8233	1.8236	1.8236	1.8866	1.8225	1.8222	1.8225	1.8151	1.815	1.8115	1.8118	1.8119
R(5,6)	1.3769	1.3461	1.3462	1.3463	1.3828	1.3474	1.3474	1.3473	1.3442	1.3441	1.3419	1.3419	1.342
A(2,1,3)	110.851	110.1903	110.1384	110.1406	110.9754	110.3332	110.2784	110.302	110.3773	110.3548	110.3342	110.3573	110.346
A(2,1,4)	109.4993	108.5507	108.5218	108.5321	109.5076	108.6005	108.6122	108.633	108.66	108.6655	108.6418	108.6594	108.6554
A(2,1,5)	110.5785	111.5649	111.5926	111.5776	110.6153	111.5188	111.5025	111.4734	111.4764	111.444	111.4636	111.4357	111.4467
A(3,1,4)	109.4932	108.556	108.5275	108.5377	109.4815	108.5982	108.6075	108.6371	108.6618	108.6733	108.6471	108.6606	108.6576
A(3,1,5)	110.5805	111.5671	111.5942	111.5793	110.5742	111.5039	111.4953	111.4453	111.4412	111.4447	111.4472	111.4267	111.4334
A(4,1,5)	105.7024	106.2474	106.3025	106.3115	105.5368	106.1169	106.1816	106.1898	106.0573	106.0954	106.1444	106.1395	106.14
A(1,5,6)	96.9622	96.9976	96.9874	96.99	96.762	96.9465	96.9295	96.919	97.1164	97.1019	97.238	97.2255	97.2349
D(2,1,5,6)	-61.5242	-61.8472	-61.8361	-61.8251	-61.6037	-61.8399	-61.8492	-61.8308	-61.79	-61.8739	-61.7764	-61.8082	-61.7875
D(3,1,5,6)	61.6437	61.8823	61.8661	61.8578	61.7438	61.9951	61.8961	61.8869	62.0251	61.8906	61.9775	61.9402	61.9593
D(4,1,5,6)	-179.9434	-179.9786	-179.9811	-179.9798	-179.9561	-179.9278	-179.9813	-179.9771	-179.8908	-179.9867	-179.9007	-179.9357	-179.9164
Energy	-438.596175548	-438.640833383	-438.642633249	-438.642747429	-438.632291442	-438.675488915	-438.676180692	-438.676513745	-438.682100484	-438.682846452	-438.686077695	-438.686356668	-438.686452209
ZPE Correction	0.046258	0.046426	0.04632	0.046306	0.045792	0.046103	0.046045	0.046067	0.045991	0.045958	0.04603	0.046014	0.046007

S4d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0972	1.0978	1.0982	1.0982	1.0925	1.0959	1.0963	1.0959	1.095	1.0953	1.0936	1.0937	1.0937
R(1,3)	1.0973	1.0978	1.0982	1.0981	1.0925	1.0959	1.0963	1.0958	1.095	1.0953	1.0937	1.0937	1.0937
R(1,4)	1.0967	1.0974	1.0978	1.0977	1.0922	1.0958	1.0961	1.0957	1.0953	1.0954	1.0939	1.094	1.094
R(1,5)	1.9161	1.8469	1.8481	1.8481	1.9198	1.8468	1.8459	1.8468	1.8388	1.8384	1.8338	1.834	1.8341
R(5,6)	1.385	1.352	1.352	1.3521	1.3902	1.3524	1.3524	1.3521	1.3487	1.3486	1.3465	1.3464	1.3465
A(2,1,3)	111.0725	110.2891	110.2601	110.2626	111.2005	110.463	110.3687	110.4433	110.4485	110.4133	110.3787	110.3912	110.385
A(2,1,4)	109.8928	108.8743	108.8653	108.873	109.9013	108.9503	108.9173	109.0152	108.9472	108.9544	108.9175	108.929	108.9262
A(2,1,5)	110.1963	111.3218	111.3419	111.3314	110.2027	111.2299	111.2421	111.2152	111.1974	111.197	111.2165	111.1973	111.2026
A(3,1,4)	109.8895	108.8573	108.8437	108.8512	109.9009	108.9314	108.911	108.9859	108.9522	108.9585	108.9235	108.9354	108.9327
A(3,1,5)	110.2012	111.274	111.2692	111.2536	110.2066	111.1701	111.224	111.0504	111.1962	111.1881	111.207	111.1894	111.1946
A(4,1,5)	105.4403	106.0827	106.1206	106.1303	105.2648	105.9495	106.0362	105.9925	105.9543	105.988	106.0575	106.0593	106.0604
A(1,5,6)	96.4028	96.7924	96.7979	96.8042	96.29	96.8218	96.8007	96.8245	97.0469	97.0258	97.1593	97.1441	97.1518
D(2,1,5,6)	-61.4362	-61.7219	-61.7002	-61.6946	-61.4945	-61.705	-61.6996	-61.6105	-61.6535	-61.6196	-61.6413	-61.6097	-61.6112
D(3,1,5,6)	61.4907	61.7435	61.7387	61.7286	61.602	61.8437	61.7749	61.8159	61.8718	61.8541	61.8153	61.8364	61.8346
D(4,1,5,6)	180.0266	-180.0123	-180.0132	-180.0171	180.0546	-179.9578	-179.971	180.0412	180.1118	180.1173	180.0881	180.115	180.1134
Energy	-438.631594287	-438.672322776	-438.675009401	-438.675097866	-438.670976818	-438.710292009	-438.710837033	-438.711108957	-438.715988053	-438.716599443	-438.720054932	-438.720261553	-438.720343089
ZPE Correction	0.0448	0.045032	0.044912	0.04489	0.044347	0.044765	0.044702	0.044721	0.044662	0.044626	0.044716	0.044699	0.044691

S4e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.092	1.0928	1.0932	1.0932	1.0872	1.091	1.0913	1.0912	1.0901	1.0903	1.0887	1.0887	1.0887
R(1,3)	1.0921	1.0927	1.0932	1.0932	1.0872	1.091	1.0913	1.0912	1.0902	1.0904	1.0887	1.0887	1.0887
R(1,4)	1.092	1.0929	1.0933	1.0933	1.0874	1.0914	1.0916	1.0915	1.091	1.0911	1.0896	1.0896	1.0896
R(1,5)	1.8982	1.8385	1.8391	1.8391	1.8999	1.8382	1.8376	1.8379	1.8293	1.829	1.826	1.8262	1.8263
R(5,6)	1.3802	1.3486	1.3487	1.3488	1.3862	1.3497	1.3495	1.3495	1.3463	1.3462	1.3435	1.3434	1.3435
A(2,1,3)	111.0418	110.3805	110.332	110.3325	111.1441	110.5356	110.4548	110.4831	110.5541	110.5241	110.5049	110.524	110.5158
A(2,1,4)	109.7334	108.8361	108.7989	108.804	109.7192	108.8938	108.8785	108.8955	108.8905	108.9029	108.8826	108.8979	108.8937
A(2,1,5)	110.3242	111.3138	111.3388	111.3284	110.3626	111.2572	111.2568	111.2129	111.2073	111.2098	111.2011	111.181	111.1873
A(3,1,4)	109.7296	108.8179	108.7849	108.7907	109.7179	108.86	108.8534	108.885	108.8886	108.8918	108.8814	108.8946	108.8913
A(3,1,5)	110.3641	111.2596	111.2989	111.2878	110.369	111.1868	111.2173	111.1792	111.2101	111.2038	111.2045	111.1833	111.1912
A(4,1,5)	105.5008	106.0852	106.1404	106.1516	105.3686	105.9529	106.0311	106.0381	105.9355	105.9564	106.0168	106.0109	106.0124
A(1,5,6)	96.772	96.927	96.9289	96.9365	96.6388	96.8738	96.8457	96.8508	97.0425	97.0245	97.1669	97.1522	97.1612
D(2,1,5,6)	-61.5503	-61.7589	-61.7051	-61.6984	-61.6325	-61.8697	-61.8354	-61.7312	-61.7913	-61.7943	-61.75	-61.7609	-61.7539
D(3,1,5,6)	61.5356	61.8086	61.8462	61.838	61.6128	61.8049	61.7564	61.8378	61.8878	61.8433	61.857	61.8409	61.8476
D(4,1,5,6)	180.0008	-180.0005	-179.9486	-179.9492	179.991	179.9286	179.9349	-179.962	-179.9521	-179.9837	-179.9464	-179.9614	-179.9535
Energy	-438.588360396	-438.631623709	-438.63379619	-438.633892997	-438.624236467	-438.666369063	-438.666984117	-438.667274706	-438.673220297	-438.673890303	-438.676869965	-438.677130056	-438.677212355
ZPE Correction	0.046041	0.046229	0.04611	0.046092	0.045581	0.04591	0.045851	0.045868	0.045829	0.045796	0.045853	0.045839	0.045834

S4f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0915	1.0925	1.0927	1.0929	1.0866	1.0906	1.0911	1.091	1.09	1.0903	1.0892	1.0892	1.0892
R(1,3)	1.0915	1.0924	1.0926	1.0929	1.0866	1.0905	1.0911	1.0909	1.09	1.0901	1.0892	1.0892	1.0892
R(1,4)	1.0912	1.0922	1.0925	1.0926	1.0865	1.0908	1.0911	1.091	1.0906	1.0907	1.0898	1.0898	1.0898
R(1,5)	1.8831	1.8175	1.8194	1.8184	1.8853	1.818	1.8173	1.8178	1.8124	1.8122	1.807	1.807	1.8071
R(5,6)	1.3774	1.3459	1.3458	1.3461	1.3841	1.3471	1.3471	1.347	1.3441	1.3439	1.3419	1.3418	1.3419
A(2,1,3)	110.7718	110.0703	110.0686	110.0164	110.9362	110.3135	110.2125	110.2303	110.3236	110.3045	110.2367	110.2407	110.2327
A(2,1,4)	109.4292	108.4101	108.4461	108.3648	109.4739	108.5555	108.5083	108.535	108.5598	108.5716	108.5172	108.5221	108.5196
A(2,1,5)	110.712	111.822	111.7944	111.8525	110.7019	111.6695	111.6749	111.6495	111.6153	111.6112	111.6562	111.6483	111.6506
A(3,1,4)	109.4239	108.4023	108.4126	108.3606	109.4668	108.5371	108.4984	108.5278	108.5468	108.6012	108.5135	108.5167	108.5155
A(3,1,5)	110.7308	111.7707	111.6919	111.8072	110.6975	111.5885	111.6688	111.6108	111.607	111.5446	111.6533	111.6447	111.6477
A(4,1,5)	105.6341	106.1805	106.2495	106.2536	105.4085	105.9941	106.0983	106.1118	106.0071	106.0325	106.0846	106.0896	106.0963
A(1,5,6)	96.8765	96.9907	97.009	97.027	96.8687	97.0671	97.0276	97.0306	97.1778	97.1388	97.3372	97.3209	97.3229
D(2,1,5,6)	-61.6509	-62.0049	-61.9535	-61.9884	-61.7291	-62.0265	-61.9692	-61.8656	-61.9765	-61.8452	-61.9402	-61.9354	-61.9342
D(3,1,5,6)	61.6137	61.9106	61.8801	61.9067	61.7152	61.9574	61.9464	62.0112	61.9941	62.051	61.9816	61.9793	61.9741
D(4,1,5,6)	-180.0168	179.9342	179.9152	179.9442	-180.0123	-180.0673	-180.019	180.058	179.9988	180.1028	180.0177	180.0177	180.0167
Energy	-438.709345302	-438.752357659	-438.755522878	-438.755616427	-438.746643595	-438.78880968	-438.789274209	-438.78950989	-438.794658803	-438.795145645	-438.79816281	-438.798320907	-438.798383667
ZPE Correction	0.045881	0.046033	0.045899	0.045875	0.045422	0.045736	0.04566	0.045666	0.045545	0.045501	0.045575	0.045564	0.045558

S4g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0906	1.0917	1.0921	1.0921	1.0858	1.09	1.0904	1.0904	1.0894	1.0897	1.0884	1.0885	1.0885
R(1,3)	1.0907	1.0917	1.0921	1.0921	1.0859	1.09	1.0905	1.0903	1.0894	1.0897	1.0884	1.0885	1.0885
R(1,4)	1.0904	1.0916	1.0919	1.092	1.0859	1.0903	1.0906	1.0905	1.09	1.0903	1.0891	1.0891	1.0891
R(1,5)	1.8875	1.8245	1.8253	1.8253	1.89	1.8246	1.8241	1.8246	1.8179	1.8175	1.8137	1.8137	1.8138
R(5,6)	1.3763	1.3451	1.3451	1.3452	1.3834	1.347	1.347	1.3469	1.344	1.3439	1.3416	1.3415	1.3416
A(2,1,3)	110.8514	110.146	110.0932	110.0922	111.0246	110.3787	110.3004	110.317	110.395	110.3639	110.3255	110.3333	110.3197
A(2,1,4)	109.5331	108.5538	108.5256	108.5314	109.5933	108.6623	108.6512	108.668	108.6831	108.6914	108.6613	108.6682	108.6634
A(2,1,5)	110.5664	111.6145	111.6431	111.6321	110.5677	111.4883	111.5038	111.4765	111.4564	111.4552	111.4735	111.4614	111.471
A(3,1,4)	109.5303	108.5444	108.511	108.5151	109.5666	108.6566	108.6436	108.6753	108.6866	108.6884	108.6633	108.6705	108.6684
A(3,1,5)	110.601	111.5936	111.6062	111.5976	110.5445	111.4814	111.4958	111.4426	111.4544	111.4516	111.474	111.4617	111.4697
A(4,1,5)	105.6202	106.2231	106.2975	106.3096	105.3874	106.0034	106.0808	106.0997	105.9974	106.0252	106.0791	106.0824	106.0854
A(1,5,6)	96.9168	97.019	97.0196	97.0265	96.8858	97.0575	97.0151	97.0096	97.1586	97.1339	97.298	97.2836	97.286
D(2,1,5,6)	-61.6277	-61.8372	-61.7537	-61.7418	-61.7387	-61.9172	-61.877	-61.8171	-61.8525	-61.8782	-61.8543	-61.8472	-61.818
D(3,1,5,6)	61.5466	61.8907	61.9359	61.9318	61.6178	61.9381	61.8983	61.9205	61.9805	61.9115	61.9153	61.9146	61.9389
D(4,1,5,6)	179.9668	-179.9846	-179.9277	-179.9242	179.9178	-179.9949	-179.9961	-179.9531	-179.9345	-179.9862	-179.9682	-179.9648	-179.9369
Energy	-438.624220456	-438.667567765	-438.670515248	-438.670619116	-438.659912922	-438.702662794	-438.703203472	-438.703472575	-438.70914144	-438.709706339	-438.712391507	-438.712549914	-438.71262538
ZPE Correction	0.046179	0.046351	0.046225	0.046201	0.045697	0.046025	0.045951	0.045958	0.045872	0.045826	0.045891	0.045875	0.045867

S4h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0985	1.099	1.0995	1.0998	1.0935	1.0972	1.0976	1.0976	1.0965	1.0966	1.0952	1.0952	1.0953
R(1,3)	1.0986	1.0989	1.0994	1.0997	1.0936	1.097	1.0975	1.0975	1.0965	1.0965	1.0952	1.0952	1.0953
R(1,4)	1.0984	1.099	1.0995	1.0997	1.0937	1.0975	1.0977	1.0977	1.0972	1.0971	1.0959	1.0959	1.096
R(1,5)	1.8983	1.8356	1.8365	1.8359	1.9021	1.8347	1.8347	1.8346	1.827	1.8268	1.8231	1.8233	1.8234
R(5,6)	1.3901	1.3576	1.3576	1.3579	1.3955	1.3583	1.3582	1.3583	1.3551	1.3548	1.3527	1.3526	1.3527
A(2,1,3)	110.974	110.332	110.2781	110.2147	111.1385	110.4659	110.3861	110.3775	110.5036	110.4868	110.4467	110.4675	110.4543
A(2,1,4)	109.558	108.6479	108.6061	108.5433	109.5866	108.647	108.6405	108.6484	108.7009	108.7233	108.6992	108.7286	108.7135
A(2,1,5)	110.5652	111.5866	111.6257	111.6533	110.5811	111.5346	111.5292	111.5231	111.4709	111.4583	111.459	111.4533	111.4522
A(3,1,4)	109.5498	108.62	108.5886	108.5314	109.5506	108.668	108.6533	108.6379	108.6877	108.7454	108.6809	108.6974	108.6888
A(3,1,5)	110.6022	111.4964	111.5254	111.6172	110.5499	111.4662	111.4916	111.4894	111.4629	111.3916	111.4471	111.3975	111.4267
A(4,1,5)	105.4392	105.9849	106.0443	106.1059	105.2646	105.8792	105.9662	105.9919	105.8354	105.8625	105.9356	105.9256	105.9338
A(1,5,6)	96.5501	96.7295	96.7424	96.7266	96.4271	96.6985	96.6405	96.6441	96.8451	96.8124	96.9652	96.947	96.9538
D(2,1,5,6)	-61.7429	-61.9236	-61.8469	-61.8534	-61.7233	-61.851	-61.862	-61.8696	-61.9799	-61.8555	-61.9387	-62.0007	-61.9601
D(3,1,5,6)	61.5875	61.9545	62.0113	62.0106	61.7915	62.1411	62.0406	62.0158	62.0117	62.0524	61.9583	61.8826	61.9268
D(4,1,5,6)	179.927	-180.0254	-179.9553	-179.9383	-179.9952	-179.8606	-179.913	-179.9422	-179.9941	-179.906	-180.0044	179.9075	179.9617
Energy	-438.407527435	-438.448746736	-438.451754406	-438.451868079	-438.446346895	-438.485853898	-438.486419628	-438.486711526	-438.492232939	-438.492853343	-438.496068614	-438.496280976	-438.496364606
ZPE Correction	0.045001	0.045192	0.04506	0.045034	0.044537	0.044878	0.044804	0.044819	0.044761	0.044724	0.044802	0.044785	0.044777

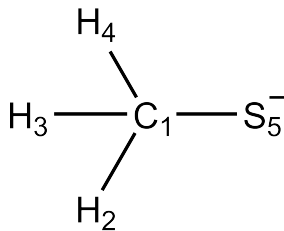
S4i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0925	1.0934	1.0937	1.0937	1.0876	1.0914	1.0915	1.0913	1.0904	1.0906	1.0888	1.0889	1.0889
R(1,3)	1.0926	1.0933	1.0937	1.0937	1.0876	1.0914	1.0914	1.0912	1.0904	1.0905	1.0888	1.0889	1.0889
R(1,4)	1.0924	1.0934	1.0937	1.0937	1.0877	1.0917	1.0917	1.0916	1.0911	1.0911	1.0896	1.0896	1.0897
R(1,5)	1.8958	1.8357	1.8363	1.8363	1.8976	1.8351	1.8344	1.8351	1.8259	1.8253	1.8227	1.8229	1.823
R(5,6)	1.3804	1.3486	1.3487	1.3488	1.3855	1.3495	1.3492	1.3491	1.3458	1.3456	1.343	1.3429	1.343
A(2,1,3)	111.0076	110.3433	110.2932	110.2941	111.1298	110.5074	110.4501	110.4979	110.5296	110.4875	110.4839	110.5048	110.4964
A(2,1,4)	109.6888	108.7865	108.7507	108.76	109.6911	108.831	108.8427	108.9054	108.8526	108.8829	108.8458	108.8643	108.8599
A(2,1,5)	110.3777	111.3761	111.4	111.3877	110.4193	111.2876	111.3049	111.2638	111.2668	111.3179	111.2507	111.2317	111.2361
A(3,1,4)	109.6864	108.7686	108.7377	108.7457	109.6697	108.8119	108.8569	108.8887	108.8468	108.8485	108.8431	108.8579	108.8556
A(3,1,5)	110.4296	111.3298	111.3675	111.3515	110.41	111.2794	111.2185	111.1401	111.2651	111.2123	111.254	111.2299	111.2377
A(4,1,5)	105.5047	106.0847	106.1407	106.1524	105.3608	105.9651	106.0166	105.9958	105.9212	105.9366	106.0105	105.9997	106.0028
A(1,5,6)	96.7019	96.8551	96.8516	96.8567	96.6139	96.8326	96.8232	96.8363	97.0488	97.0375	97.1473	97.1333	97.143
D(2,1,5,6)	-61.5533	-61.7858	-61.7369	-61.7212	-61.7031	-61.9741	-61.6622	-61.6755	-61.8429	-61.895	-61.7931	-61.8017	-61.7937
D(3,1,5,6)	61.5708	61.8299	61.8587	61.8548	61.5914	61.7533	61.9592	61.9212	61.8877	61.7798	61.8585	61.8457	61.8516
D(4,1,5,6)	-179.9793	179.9989	180.0443	180.0485	-180.0709	-180.124	-179.8661	180.0798	180.0184	-180.1063	180.032	180.0177	180.0268
Energy	-438.611081909	-438.653800128	-438.655862357	-438.655962195	-438.648904061	-438.689894186	-438.690543307	-438.690847702	-438.696531938	-438.697244075	-438.700714258	-438.700978828	-438.701063689
ZPE Correction	0.045857	0.045985	0.045876	0.045859	0.045406	0.045682	0.045627	0.045645	0.045617	0.045587	0.045641	0.045627	0.04562

S4j – QCISD

	QCISD/cc-pVTZ
R(1,2)	1.0865
R(1,3)	1.0865
R(1,4)	1.0875
R(1,5)	1.8211
R(5,6)	1.3389
A(2,1,3)	110.2918
A(2,1,4)	108.8224
A(2,1,5)	111.2312
A(3,1,4)	108.8113
A(3,1,5)	111.2152
A(4,1,5)	106.3357
A(1,5,6)	96.812
D(2,1,5,6)	-61.6376
D(3,1,5,6)	61.7232
D(4,1,5,6)	180.0317
Energy	-438.1538405
ZPE Correction	0.046473

S5 – MeS[−]



S5a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1015	1.1029	1.1002	1.1005	1.0942	1.0985	1.0984	1.0984	1.0972	1.0971	1.0957	1.0953	1.0954
R(1,3)	1.1015	1.1029	1.1002	1.1005	1.0942	1.0985	1.0984	1.0984	1.0972	1.0971	1.0957	1.0953	1.0954
R(1,4)	1.1015	1.1029	1.1002	1.1005	1.0942	1.0985	1.0984	1.0984	1.0972	1.0971	1.0957	1.0953	1.0954
R(1,5)	1.9029	1.8432	1.8519	1.8511	1.9164	1.8491	1.8483	1.8485	1.8429	1.8423	1.8393	1.8389	1.8388
A(2,1,3)	107.5125	106.1686	106.9912	106.9707	108.2605	106.991	107.062	107.0685	107.0365	107.145	107.0956	107.1964	107.1861
A(2,1,4)	107.5125	106.1686	106.9912	106.9707	108.2605	106.991	107.062	107.0685	107.0365	107.145	107.0956	107.1964	107.1861
A(2,1,5)	111.3654	112.6006	111.85	111.869	110.6564	111.8502	111.7846	111.7786	111.8082	111.7078	111.7535	111.6601	111.6696
A(3,1,4)	107.5125	106.1686	106.9912	106.9707	108.2605	106.991	107.062	107.0685	107.0365	107.145	107.0956	107.1964	107.1861
A(3,1,5)	111.3654	112.6006	111.85	111.869	110.6564	111.8502	111.7846	111.7786	111.8082	111.7078	111.7535	111.6601	111.6696
A(4,1,5)	111.3654	112.6006	111.85	111.869	110.6564	111.8502	111.7846	111.7786	111.8082	111.7078	111.7535	111.6601	111.6696
D(2,1,4,3)	115.4953	112.7016	114.3859	114.3427	117.1499	114.3854	114.5345	114.5482	114.4809	114.7096	114.6054	114.8184	114.7967
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.086563376	-438.114105663	-438.134001655	-438.134123579	-438.140792824	-438.166179964	-438.168216196	-438.168294481	-438.170772576	-438.172729988	-438.173771794	-438.175443071	-438.175514243
ZPE Correction	0.036238	0.035959	0.035958	0.035882	0.036047	0.035831	0.035761	0.035737	0.035837	0.035783	0.035806	0.035817	0.035786

S5b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1012	1.1024	1.1002	1.1005	1.0944	1.0988	1.0989	1.0988	1.0977	1.0977	1.0964	1.0962	1.0963
R(1,3)	1.1012	1.1024	1.1002	1.1005	1.0944	1.0988	1.0989	1.0988	1.0977	1.0977	1.0964	1.0962	1.0963
R(1,4)	1.1012	1.1024	1.1002	1.1005	1.0944	1.0988	1.0989	1.0988	1.0977	1.0977	1.0964	1.0962	1.0963
R(1,5)	1.886	1.8284	1.8362	1.8355	1.897	1.8339	1.8329	1.8331	1.8276	1.8267	1.8225	1.8234	1.8233
A(2,1,3)	107.3939	106.0927	106.8395	106.8157	108.0814	106.8741	106.9104	106.9229	106.9047	106.9802	106.9034	107.0101	107.0011
A(2,1,4)	107.3939	106.0927	106.8395	106.8157	108.0814	106.8741	106.9104	106.9229	106.9047	106.9802	106.9034	107.0101	107.0011
A(2,1,5)	111.4762	112.669	111.9898	112.0116	110.8277	111.9579	111.9245	111.913	111.9297	111.8602	111.9309	111.8326	111.8409
A(3,1,4)	107.3939	106.0927	106.8395	106.8157	108.0814	106.8741	106.9104	106.9229	106.9047	106.9802	106.9034	107.0101	107.0011
A(3,1,5)	111.4762	112.669	111.9898	112.0116	110.8277	111.9579	111.9245	111.913	111.9297	111.8602	111.9309	111.8326	111.8409
A(4,1,5)	111.4762	112.669	111.9898	112.0116	110.8277	111.9579	111.9245	111.913	111.9297	111.8602	111.9309	111.8326	111.8409
D(2,1,4,3)	115.24	112.5503	114.0691	114.0197	116.7467	114.1412	114.2169	114.2428	114.205	114.3627	114.2023	114.4254	114.4066
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.572882698	-438.60035844	-438.615861493	-438.615970957	-438.621754192	-438.647655896	-438.649093287	-438.649185335	-438.65244983	-438.653808586	-438.655209512	-438.656318806	-438.656388544
ZPE Correction	0.036443	0.036112	0.036105	0.03604	0.036258	0.035961	0.035898	0.035885	0.035942	0.035896	0.035915	0.035911	0.035889

S5c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1014	1.1031	1.1009	1.1012	1.0953	1.0997	1.0997	1.0997	1.0986	1.0986	1.0975	1.0971	1.0972
R(1,3)	1.1014	1.1031	1.1009	1.1012	1.0953	1.0997	1.0997	1.0997	1.0986	1.0986	1.0975	1.0971	1.0972
R(1,4)	1.1014	1.1031	1.1009	1.1012	1.0953	1.0997	1.0997	1.0997	1.0986	1.0986	1.0975	1.0971	1.0972
R(1,5)	1.8897	1.8308	1.8383	1.8375	1.8993	1.836	1.8349	1.8352	1.8298	1.8289	1.8246	1.8256	1.8241
A(2,1,3)	107.4978	106.113	106.8526	106.8273	108.0813	106.8733	106.9103	106.922	106.9033	106.9844	106.8946	107.0126	106.9629
A(2,1,4)	107.4978	106.113	106.8526	106.8273	108.0813	106.8733	106.9103	106.922	106.9033	106.9844	106.8946	107.0126	106.9629
A(2,1,5)	111.3791	112.6507	111.9777	112.0009	110.8277	111.9586	111.9246	111.9138	111.9311	111.8563	111.939	111.8302	111.8762
A(3,1,4)	107.4978	106.113	106.8526	106.8273	108.0813	106.8733	106.9103	106.922	106.9033	106.9844	106.8946	107.0126	106.9629
A(3,1,5)	111.3791	112.6507	111.9777	112.0009	110.8277	111.9586	111.9246	111.9138	111.9311	111.8563	111.939	111.8302	111.8762
A(4,1,5)	111.3791	112.6507	111.9777	112.0009	110.8277	111.9586	111.9246	111.9138	111.9311	111.8563	111.939	111.8302	111.8762
D(2,1,4,3)	115.4637	112.5908	114.0964	114.0439	116.7465	114.1395	114.2167	114.2411	114.202	114.3715	114.1839	114.4307	114.3264
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.022413758	-438.049691311	-438.065199664	-438.065305675	-438.070706224	-438.096462042	-438.098047331	-438.098151942	-438.10126521	-438.102773118	-438.103966244	-438.10516367	-438.10524584
ZPE Correction	0.036418	0.036073	0.036065	0.035992	0.036203	0.035911	0.035843	0.035824	0.035887	0.035838	0.035858	0.035851	0.03583

S5d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1108	1.1119	1.1081	1.1085	1.1035	1.1068	1.1066	1.1067	1.1055	1.1053	1.1043	1.1037	1.1039
R(1,3)	1.1108	1.1119	1.1081	1.1085	1.1035	1.1068	1.1066	1.1067	1.1055	1.1053	1.1043	1.1037	1.1039
R(1,4)	1.1108	1.1119	1.1081	1.1086	1.1035	1.1068	1.1066	1.1068	1.1055	1.1053	1.1043	1.1037	1.104
R(1,5)	1.9136	1.8494	1.8602	1.8593	1.9304	1.8567	1.8562	1.8563	1.8508	1.8504	1.8466	1.8465	1.8464
A(2,1,3)	107.3003	105.8787	106.7709	106.7489	108.1233	106.7358	106.8381	106.8423	106.7955	106.9429	106.8468	106.9905	106.9781
A(2,1,4)	107.3003	105.8787	106.7709	106.7476	108.1233	106.7358	106.8381	106.8487	106.7955	106.9429	106.8468	106.9905	106.9799
A(2,1,5)	111.5635	112.8612	112.0527	112.0706	110.7877	112.0849	111.991	111.9816	112.0301	111.8946	111.983	111.8507	111.8602
A(3,1,4)	107.3003	105.8787	106.7709	106.7511	108.1233	106.7358	106.8381	106.8554	106.7955	106.9429	106.8468	106.9905	106.9878
A(3,1,5)	111.5635	112.8612	112.0527	112.0679	110.7877	112.0849	111.991	111.9762	112.0301	111.8946	111.983	111.8507	111.8534
A(4,1,5)	111.5635	112.8612	112.0527	112.0794	110.7877	112.0849	111.991	111.9857	112.0301	111.8946	111.983	111.8507	111.8623
D(2,1,4,3)	115.0395	112.1267	113.9269	113.8818	116.8406	113.8544	114.0662	114.0842	113.978	114.2846	114.0843	114.3842	114.3637
D(2,1,5,3)	-120	-120	-120	-119.9948	-120	-120	-120	-119.9885	-120	-120	-120	-120	-119.9925
D(2,1,5,4)	120	120	120	120.0012	120	120	120	120.0033	120	120	120	120	120.0011
D(3,1,5,4)	-120	-120	-120	-120.0039	-120	-120	-120	-120.0082	-120	-120	-120	-120	-120.0064
Energy	-438.051337954	-438.076597454	-438.096761515	-438.096886446	-438.106302657	-438.129658195	-438.132048872	-438.132130839	-438.133788019	-438.136144304	-438.136716248	-438.138637052	-438.138717316
ZPE Correction	0.035046	0.034762	0.034835	0.034721	0.034882	0.034697	0.03464	0.034588	0.034685	0.034646	0.034644	0.034663	0.034607

S5e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.103	1.1043	1.1018	1.1021	1.0964	1.1003	1.1003	1.1002	1.0992	1.0991	1.0979	1.0975	1.0976
R(1,3)	1.103	1.1043	1.1018	1.1021	1.0964	1.1003	1.1003	1.1002	1.0992	1.0991	1.0979	1.0975	1.0976
R(1,4)	1.103	1.1043	1.1018	1.1021	1.0964	1.1003	1.1003	1.1002	1.0992	1.0991	1.0979	1.0975	1.0976
R(1,5)	1.9025	1.8449	1.853	1.8523	1.9125	1.8506	1.8498	1.85	1.8435	1.8429	1.8405	1.8402	1.8401
A(2,1,3)	107.6027	106.294	107.0444	107.028	108.2431	107.0539	107.1146	107.1224	107.1012	107.1997	107.1541	107.2483	107.2408
A(2,1,4)	107.6027	106.294	107.0444	107.028	108.2431	107.0539	107.1146	107.1224	107.1012	107.1997	107.1541	107.2483	107.2408
A(2,1,5)	111.2807	112.4873	111.8009	111.8161	110.6731	111.7921	111.736	111.7287	111.7483	111.657	111.6993	111.6119	111.6189
A(3,1,4)	107.6027	106.294	107.0444	107.028	108.2431	107.0539	107.1146	107.1224	107.1012	107.1997	107.1541	107.2483	107.2408
A(3,1,5)	111.2807	112.4873	111.8009	111.8161	110.6731	111.7921	111.736	111.7287	111.7483	111.657	111.6993	111.6119	111.6189
A(4,1,5)	111.2807	112.4873	111.8009	111.8161	110.6731	111.7921	111.736	111.7287	111.7483	111.657	111.6993	111.6119	111.6189
D(2,1,4,3)	115.6909	112.9533	114.4975	114.463	117.1104	114.5174	114.6453	114.6619	114.6171	114.8255	114.7289	114.9288	114.9128
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.014583683	-438.040784942	-438.058209169	-438.058311861	-438.063907394	-438.088852443	-438.090737137	-438.090819453	-438.093714677	-438.095515846	-438.096230958	-438.097726541	-438.097793091
ZPE Correction	0.036251	0.035924	0.03593	0.035861	0.036068	0.035794	0.035727	0.035708	0.035785	0.035735	0.035738	0.035748	0.035723

S5f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1041	1.1056	1.1025	1.103	1.0969	1.1016	1.1014	1.1015	1.1009	1.1006	1.1006	1.0995	1.0997
R(1,3)	1.1041	1.1056	1.1025	1.103	1.0969	1.1016	1.1014	1.1015	1.1009	1.1006	1.1006	1.0995	1.0997
R(1,4)	1.1041	1.1056	1.1025	1.103	1.0969	1.1016	1.1014	1.1015	1.1009	1.1006	1.1006	1.0995	1.0997
R(1,5)	1.8808	1.8198	1.8293	1.8281	1.8932	1.8255	1.8263	1.8261	1.8205	1.8217	1.8148	1.8171	1.8165
A(2,1,3)	106.9682	105.5484	106.4402	106.3863	107.7621	106.4029	106.5386	106.5336	106.3899	106.5992	106.3684	106.6085	106.5881
A(2,1,4)	106.9682	105.5484	106.4402	106.3981	107.7621	106.4029	106.5386	106.5336	106.3899	106.5992	106.3684	106.6085	106.5881
A(2,1,5)	111.8713	113.1558	112.3547	112.3974	111.1306	112.3885	112.2651	112.2696	112.4003	112.2098	112.4199	112.2013	112.2199
A(3,1,4)	106.9682	105.5484	106.4402	106.3987	107.7621	106.4029	106.5386	106.5336	106.3899	106.5992	106.3684	106.6085	106.5881
A(3,1,5)	111.8713	113.1558	112.3547	112.3947	111.1306	112.3885	112.2651	112.2696	112.4003	112.2098	112.4199	112.2013	112.2199
A(4,1,5)	111.8713	113.1558	112.3547	112.3967	111.1306	112.3885	112.2651	112.2696	112.4003	112.2098	112.4199	112.2013	112.2199
D(2,1,4,3)	114.3376	111.4825	113.249	113.1505	116.039	113.1733	113.4494	113.4392	113.1471	113.5733	113.1035	113.5925	113.5506
D(2,1,5,3)	-120	-120	-120	-119.9892	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120.006	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120.0048	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.128880196	-438.155568582	-438.177011996	-438.177130018	-438.181293299	-438.206742917	-438.210415975	-438.210491742	-438.210951006	-438.21448048	-438.21400901	-438.216777259	-438.21686002
ZPE Correction	0.035996	0.035638	0.035644	0.035523	0.035832	0.035522	0.035429	0.035376	0.035441	0.035368	0.03535	0.03538	0.03533

S5g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1021	1.1037	1.1012	1.1018	1.0959	1.1003	1.1004	1.1006	1.0996	1.0996	1.0989	1.0983	1.0985
R(1,3)	1.1021	1.1037	1.1012	1.1018	1.0959	1.1003	1.1004	1.1006	1.0996	1.0996	1.0989	1.0983	1.0985
R(1,4)	1.1021	1.1037	1.1012	1.1018	1.0959	1.1003	1.1004	1.1006	1.0996	1.0996	1.0989	1.0983	1.0985
R(1,5)	1.8896	1.8295	1.838	1.8354	1.8983	1.8333	1.833	1.8329	1.8272	1.8272	1.8228	1.8238	1.8232
A(2,1,3)	107.3136	105.905	106.7171	106.6297	107.9067	106.6338	106.719	106.7154	106.6273	106.7839	106.6347	106.8056	106.7807
A(2,1,4)	107.3136	105.905	106.7171	106.6297	107.9067	106.6338	106.719	106.7154	106.6273	106.7839	106.6347	106.8056	106.7807
A(2,1,5)	111.5511	112.8377	112.102	112.1819	110.9937	112.1782	112.1002	112.1035	112.1841	112.0408	112.1774	112.0209	112.0437
A(3,1,4)	107.3136	105.905	106.7171	106.6297	107.9067	106.6338	106.719	106.7154	106.6273	106.7839	106.6347	106.8056	106.7807
A(3,1,5)	111.5511	112.8377	112.102	112.1819	110.9937	112.1782	112.1002	112.1035	112.1841	112.0408	112.1774	112.0209	112.0437
A(4,1,5)	111.5511	112.8377	112.102	112.1819	110.9937	112.1782	112.1002	112.1035	112.1841	112.0408	112.1774	112.0209	112.0437
D(2,1,4,3)	115.068	112.1783	113.8157	113.6359	116.3579	113.6443	113.8198	113.8123	113.631	113.9539	113.6462	113.9988	113.9472
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.04623434	-438.07257091	-438.091801784	-438.091936814	-438.095244984	-438.120809393	-438.123789579	-438.123895096	-438.125414077	-438.128288234	-438.12808293	-438.130302433	-438.130410609
ZPE Correction	0.036297	0.035944	0.035917	0.035799	0.036094	0.035791	0.035688	0.035627	0.035729	0.03565	0.035654	0.035657	0.035599

S5h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1109	1.1122	1.1091	1.1095	1.104	1.1079	1.1075	1.1076	1.1069	1.1067	1.1059	1.1052	1.1055
R(1,3)	1.1109	1.1122	1.1091	1.1095	1.104	1.1079	1.1075	1.1076	1.1069	1.1067	1.1059	1.1052	1.1054
R(1,4)	1.1109	1.1122	1.1091	1.1096	1.104	1.1079	1.1075	1.1076	1.1069	1.1067	1.1059	1.1052	1.1054
R(1,5)	1.8973	1.8388	1.8499	1.8487	1.9113	1.8449	1.8461	1.8462	1.8381	1.8381	1.8341	1.8347	1.8343
A(2,1,3)	107.2098	105.8004	106.777	106.7421	107.9751	106.6809	106.832	106.8309	106.7068	106.8668	106.7323	106.9067	106.8952
A(2,1,4)	107.2098	105.8004	106.777	106.7412	107.9751	106.6809	106.832	106.8395	106.7068	106.8668	106.7323	106.9067	106.8825
A(2,1,5)	111.6476	112.9313	112.0471	112.0761	110.9289	112.1351	111.9966	111.9922	112.1115	111.9646	112.0881	111.9279	111.9498
A(3,1,4)	107.2098	105.8004	106.777	106.7297	107.9751	106.6809	106.832	106.8485	106.7068	106.8668	106.7323	106.9067	106.8954
A(3,1,5)	111.6476	112.9313	112.0471	112.0837	110.9289	112.1351	111.9966	111.9925	112.1115	111.9646	112.0881	111.9279	111.9318
A(4,1,5)	111.6476	112.9313	112.0471	112.0897	110.9289	112.1351	111.9966	111.9841	112.1115	111.9646	112.0881	111.9279	111.9453
D(2,1,4,3)	114.847	111.9729	113.9396	113.8613	116.5095	113.7412	114.0536	114.0635	113.7945	114.126	113.8471	114.2092	114.1792
D(2,1,5,3)	-120	-120	-120	-120.0011	-120	-120	-120	-119.9926	-120	-120	-120	-120	-120.0033
D(2,1,5,4)	120	120	120	120.0041	120	120	120	119.9978	120	120	120	120	119.9963
D(3,1,5,4)	-120	-120	-120	-119.9947	-120	-120	-120	-120.0096	-120	-120	-120	-120	-120.0004
Energy	-437.833442522	-437.859131395	-437.87950801	-437.879653345	-437.887424182	-437.911013035	-437.913557134	-437.913649124	-437.915585251	-437.91806977	-437.918429671	-437.920464852	-437.920556284
ZPE Correction	0.035306	0.034957	0.034979	0.034873	0.035143	0.034841	0.034765	0.03472	0.034812	0.034757	0.034764	0.034777	0.034726

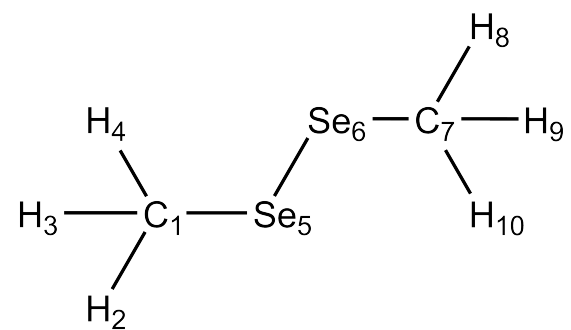
S5i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1043	1.1058	1.1027	1.103	1.0974	1.101	1.101	1.101	1.1002	1.1001	1.0988	1.0984	1.0985
R(1,3)	1.1043	1.1058	1.1027	1.103	1.0974	1.101	1.101	1.101	1.1002	1.1001	1.0988	1.0984	1.0985
R(1,4)	1.1043	1.1058	1.1027	1.103	1.0974	1.101	1.101	1.101	1.1002	1.1001	1.0988	1.0984	1.0985
R(1,5)	1.8987	1.8407	1.8499	1.8492	1.909	1.8473	1.8464	1.8466	1.8392	1.8385	1.836	1.8357	1.8356
A(2,1,3)	107.4822	106.1447	106.9682	106.9509	108.1628	107.0112	107.0609	107.0697	107.0166	107.1107	107.0613	107.1516	107.1413
A(2,1,4)	107.4822	106.1447	106.9682	106.9509	108.1628	107.0112	107.0609	107.0697	107.0166	107.1107	107.0613	107.1516	107.1413
A(2,1,5)	111.3937	112.6222	111.8712	111.8872	110.7499	111.8316	111.7857	111.7775	111.8266	111.7396	111.7852	111.7017	111.7112
A(3,1,4)	107.4822	106.1447	106.9682	106.9509	108.1628	107.0112	107.0609	107.0697	107.0166	107.1107	107.0613	107.1516	107.1413
A(3,1,5)	111.3937	112.6222	111.8712	111.8872	110.7499	111.8316	111.7857	111.7775	111.8266	111.7396	111.7852	111.7017	111.7112
A(4,1,5)	111.3937	112.6222	111.8712	111.8872	110.7499	111.8316	111.7857	111.7775	111.8266	111.7396	111.7852	111.7017	111.7112
D(2,1,4,3)	115.4299	112.6539	114.3376	114.3013	116.9295	114.4277	114.5321	114.5506	114.4391	114.637	114.5331	114.7235	114.7018
D(2,1,5,3)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
D(2,1,5,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(3,1,5,4)	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120	-120
Energy	-438.035984453	-438.06226972	-438.079063406	-438.079174957	-438.087222754	-438.111586126	-438.113235361	-438.113329207	-438.116294757	-438.11788902	-438.119234052	-438.120519954	-438.120591903
ZPE Correction	0.036044	0.035704	0.035742	0.035668	0.035866	0.035611	0.035543	0.035523	0.035598	0.035549	0.035565	0.035571	0.035542

S5j – QCISD

	QCISD/cc-pVTZ
R(1,2)	1.0972
R(1,3)	1.0972
R(1,4)	1.0972
R(1,5)	1.8363
A(2,1,3)	106.6295
A(2,1,4)	106.6295
A(2,1,5)	112.1821
A(3,1,4)	106.6295
A(3,1,5)	112.1821
A(4,1,5)	112.1821
D(2,1,4,3)	113.6356
D(2,1,5,3)	-120
D(2,1,5,4)	120
D(3,1,5,4)	-120
Energy	-437.5627041
ZPE Correction	0.036139

S6 – MeSeSeMe



S6a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0889	1.0891	1.0904	1.0903	1.0851	1.0877	1.0877	1.0877	1.0866	1.0867	1.085	1.0849	1.085
R(1,3)	1.0882	1.0888	1.09	1.0899	1.0848	1.0874	1.0875	1.0875	1.0864	1.0865	1.0848	1.0848	1.0848
R(1,4)	1.0919	1.0926	1.0938	1.0935	1.0887	1.0915	1.0917	1.0917	1.0904	1.0905	1.0888	1.0888	1.0888
R(1,5)	2.0038	1.977	1.9719	1.9775	1.9968	1.9809	1.9809	1.981	1.9734	1.9734	1.9731	1.9733	1.9733
R(5,6)	2.4315	2.3302	2.3334	2.3311	2.438	2.3548	2.3546	2.3546	2.3404	2.3406	2.341	2.3411	2.3411
R(6,7)	2.0038	1.977	1.9719	1.9775	1.9968	1.9809	1.9809	1.981	1.9734	1.9735	1.9731	1.9733	1.9733
R(7,8)	1.0919	1.0926	1.0938	1.0935	1.0887	1.0915	1.0917	1.0917	1.0904	1.0905	1.0888	1.0888	1.0888
R(7,9)	1.0889	1.0891	1.0904	1.0903	1.0851	1.0877	1.0877	1.0877	1.0866	1.0867	1.085	1.0849	1.085
R(7,10)	1.0882	1.0888	1.09	1.0899	1.0848	1.0874	1.0875	1.0875	1.0864	1.0865	1.0848	1.0848	1.0848
A(2,1,3)	111.472	111.2685	110.5947	111.0089	110.7878	110.99	111.0114	111.0145	110.9189	110.9494	110.9661	111.0095	111.0107
A(2,1,4)	110.0835	109.8133	109.5237	109.7679	109.816	109.8422	109.8281	109.8349	109.8048	109.8011	109.8356	109.8563	109.8587
A(2,1,5)	109.4109	110.0702	110.5932	110.0271	110.4019	110.4026	110.4215	110.4128	110.4348	110.4493	110.3989	110.3779	110.3763
A(3,1,4)	110.4455	110.0181	109.7589	110.1208	109.9394	110.0048	109.9963	110.001	109.9867	109.9851	110.0098	110.0304	110.0331
A(3,1,5)	108.3681	109.2205	110.0328	109.2222	109.6612	109.6701	109.6873	109.6721	109.7079	109.7094	109.6746	109.6468	109.6424
A(4,1,5)	106.9337	106.327	106.2421	106.5939	106.1293	105.8032	105.7655	105.775	105.8661	105.8215	105.8304	105.7905	105.7902
A(1,5,6)	95.1651	100.3165	100.7448	100.5578	100.0954	101.2411	101.281	101.2804	101.3686	101.4282	101.4286	101.4409	101.4422
A(5,6,7)	95.1638	100.3189	100.7453	100.5615	100.0967	101.2409	101.281	101.2803	101.3683	101.428	101.4285	101.441	101.4422
A(6,7,8)	106.9333	106.3255	106.2421	106.5882	106.128	105.8032	105.7654	105.7749	105.8662	105.8215	105.8303	105.7904	105.7902
A(6,7,9)	109.409	110.0725	110.5914	110.031	110.4006	110.4009	110.4199	110.4113	110.4329	110.4474	110.3969	110.3759	110.3743
A(6,7,10)	108.3664	109.223	110.0339	109.226	109.6627	109.6711	109.6884	109.6731	109.709	109.7106	109.676	109.6484	109.6438
A(8,7,9)	110.0845	109.8121	109.5224	109.7662	109.8145	109.8418	109.8276	109.8345	109.8044	109.8007	109.8351	109.8557	109.8582
A(8,7,10)	110.4469	110.0167	109.7601	110.1195	109.9413	110.0054	109.9969	110.0016	109.9874	109.9858	110.0105	110.0312	110.0339
A(9,7,10)	111.4733	111.2678	110.5953	111.0095	110.7884	110.9905	111.0118	111.0149	110.9193	110.9498	110.9665	111.0099	111.011
D(2,1,5,6)	-66.2591	-69.0627	-63.776	-72.7166	-65.423	-65.5318	-65.5469	-65.5684	-65.3388	-65.3346	-65.2181	-65.1808	-65.2247
D(3,1,5,6)	55.4725	53.3739	58.7013	49.3706	56.9205	57.0718	57.1076	57.0739	57.2221	57.2752	57.3559	57.4153	57.3688
D(4,1,5,6)	174.5403	172.0518	177.453	168.3205	175.6256	175.6751	175.6887	175.658	175.859	175.8859	175.9827	176.0297	175.984
D(1,5,6,7)	85.0766	87.0424	88.4432	84.8146	87.6572	88.2598	88.2249	88.176	88.2061	88.3699	88.4034	88.3544	88.345
D(5,6,7,8)	174.5515	172.0661	177.4828	168.3916	175.6759	175.6844	175.6992	175.6675	175.867	175.8935	175.9926	176.0424	175.995
D(5,6,7,9)	-66.2479	-69.0495	-63.7486	-72.6486	-65.3758	-65.5238	-65.5378	-65.5604	-65.3322	-65.3284	-65.21	-65.1699	-65.2153
D(5,6,7,10)	55.4831	53.3893	58.7291	49.4444	56.9685	57.0798	57.1169	57.0821	57.2286	57.2814	57.3642	57.4263	57.3783
Energy	-4878.14992582	-4878.61746119	-4878.65495273	-4878.65736193	-4882.88998416	-4882.97040434	-4882.9714416	-4882.97154393	-4882.97474636	-4882.97581395	-4882.98594839	-4882.98667798	-4882.98672945
ZPE Correction	0.076516	0.075451	0.075504	0.075176	0.075659	0.074827	0.074787	0.074785	0.074774	0.074755	0.074868	0.074855	0.074855

S6b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0887	1.0889	1.09	1.09	1.0854	1.0878	1.0879	1.0879	1.0869	1.087	1.0854	1.0854	1.0854
R(1,3)	1.0881	1.0886	1.0897	1.0897	1.0851	1.0876	1.0877	1.0877	1.0868	1.0868	1.0853	1.0853	1.0853
R(1,4)	1.0915	1.0923	1.0934	1.093	1.0889	1.0917	1.0918	1.0918	1.0906	1.0907	1.0892	1.0892	1.0892
R(1,5)	1.984	1.9576	1.952	1.9573	1.9765	1.9614	1.9613	1.9613	1.9543	1.9542	1.954	1.9541	1.9541
R(5,6)	2.4083	2.3058	2.3086	2.3063	2.4113	2.3285	2.3283	2.3283	2.3144	2.3144	2.315	2.315	2.315
R(6,7)	1.9841	1.9576	1.952	1.9573	1.9765	1.9614	1.9613	1.9613	1.9543	1.9542	1.954	1.9541	1.9541
R(7,8)	1.0915	1.0923	1.0934	1.093	1.0889	1.0917	1.0918	1.0918	1.0906	1.0907	1.0892	1.0892	1.0892
R(7,9)	1.0887	1.0889	1.09	1.09	1.0854	1.0878	1.0879	1.0879	1.0869	1.087	1.0854	1.0854	1.0854
R(7,10)	1.0881	1.0887	1.0897	1.0897	1.0851	1.0876	1.0877	1.0877	1.0868	1.0868	1.0853	1.0853	1.0853
A(2,1,3)	111.3408	111.2248	110.4826	110.8954	110.5991	110.9258	110.9277	110.933	110.8703	110.8844	110.9047	110.9347	110.9368
A(2,1,4)	109.8778	109.6812	109.3378	109.6002	109.593	109.6813	109.6607	109.669	109.6608	109.6502	109.6902	109.7057	109.7083
A(2,1,5)	109.5855	110.2173	110.7522	110.2071	110.6005	110.5665	110.5896	110.5813	110.5733	110.5963	110.5291	110.5171	110.5152
A(3,1,4)	110.2714	109.8673	109.587	109.9492	109.7372	109.8382	109.8252	109.8301	109.8427	109.8326	109.8633	109.8777	109.8806
A(3,1,5)	108.4599	109.2595	110.1627	109.2969	109.8424	109.7715	109.795	109.7771	109.7749	109.7858	109.7428	109.7231	109.7189
A(4,1,5)	107.2024	106.476	106.4285	106.8051	106.3781	105.9365	105.9204	105.9286	106.0033	105.9739	105.9935	105.9627	105.9612
A(1,5,6)	94.8736	100.2514	100.5582	100.3999	99.7325	101.0746	101.1064	101.1072	101.1892	101.2415	101.2363	101.2448	101.2494
A(5,6,7)	94.8717	100.2559	100.5592	100.4017	99.7347	101.0728	101.1049	101.1057	101.1873	101.2398	101.2353	101.2439	101.2484
A(6,7,8)	107.2032	106.4731	106.4284	106.8037	106.377	105.9377	105.9213	105.9295	106.0045	105.975	105.994	105.9632	105.9617
A(6,7,9)	109.5823	110.2207	110.7492	110.2084	110.5995	110.5654	110.5884	110.5801	110.5725	110.5955	110.5277	110.5154	110.5137
A(6,7,10)	108.4573	109.2641	110.1648	109.2984	109.8448	109.7701	109.7942	109.7762	109.7734	109.7844	109.7429	109.7235	109.719
A(8,7,9)	109.8794	109.6791	109.3358	109.5998	109.5919	109.6815	109.6608	109.669	109.661	109.6504	109.6899	109.7053	109.708
A(8,7,10)	110.2736	109.865	109.5889	109.9485	109.738	109.8389	109.826	109.8308	109.8432	109.8331	109.864	109.8785	109.8813
A(9,7,10)	111.3418	111.224	110.4835	110.895	110.599	110.9262	110.9282	110.9334	110.8707	110.8848	110.9051	110.9351	110.9371
D(2,1,5,6)	-66.8579	-70.1861	-63.894	-73.0478	-64.9043	-65.7328	-65.767	-65.7975	-65.5337	-65.596	-65.3596	-65.3587	-65.3994
D(3,1,5,6)	54.8769	52.3169	58.6373	49.0626	57.4548	56.9673	56.9669	56.9253	57.1033	57.0815	57.2696	57.287	57.2447
D(4,1,5,6)	173.9362	170.9203	177.3613	167.9682	176.1573	175.5014	175.4888	175.4482	175.6822	175.6375	175.8505	175.8573	175.8154
D(1,5,6,7)	84.8532	86.8025	88.1925	84.5835	87.4076	88.1694	88.1843	88.1305	88.129	88.3174	88.3449	88.3232	88.3177
D(5,6,7,8)	173.9392	170.948	177.4104	167.9909	176.2033	175.4855	175.4789	175.4374	175.6619	175.617	175.846	175.8564	175.8117
D(5,6,7,9)	-66.8542	-70.1607	-63.8489	-73.0256	-64.8609	-65.7483	-65.777	-65.8083	-65.5534	-65.616	-65.3649	-65.3607	-65.4039
D(5,6,7,10)	54.8782	52.3465	58.683	49.0861	57.4991	56.9507	56.9561	56.9136	57.0825	57.0605	57.2639	57.2846	57.2398
Energy	-4880.03895221	-4880.50667154	-4880.54218261	-4880.54450934	-4884.78164	-4884.86360385	-4884.86440692	-4884.86454583	-4884.86822537	-4884.8690105	-4884.87931208	-4884.87980587	-4884.87986503
ZPE Correction	0.07696	0.07574	0.075822	0.075507	0.076052	0.075091	0.075061	0.075062	0.074983	0.074976	0.075073	0.075062	0.075059

S6c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0892	1.0895	1.0906	1.0906	1.0861	1.0885	1.0886	1.0886	1.0876	1.0877	1.0863	1.0862	1.0862
R(1,3)	1.0887	1.0893	1.0903	1.0903	1.0859	1.0883	1.0884	1.0884	1.0875	1.0876	1.0861	1.0861	1.0861
R(1,4)	1.0922	1.093	1.094	1.0937	1.0897	1.0924	1.0925	1.0925	1.0914	1.0916	1.09	1.09	1.0901
R(1,5)	1.9873	1.9608	1.9551	1.9604	1.9801	1.9648	1.9647	1.9647	1.9577	1.9577	1.9573	1.9574	1.9575
R(5,6)	2.4126	2.3085	2.3112	2.3089	2.4152	2.3316	2.3314	2.3314	2.318	2.318	2.3184	2.3184	2.3184
R(6,7)	1.9874	1.9608	1.9552	1.9604	1.9801	1.9648	1.9647	1.9647	1.9577	1.9577	1.9573	1.9574	1.9575
R(7,8)	1.0922	1.093	1.094	1.0937	1.0897	1.0924	1.0925	1.0925	1.0914	1.0916	1.09	1.09	1.0901
R(7,9)	1.0892	1.0895	1.0906	1.0906	1.0861	1.0885	1.0886	1.0886	1.0876	1.0877	1.0863	1.0862	1.0862
R(7,10)	1.0887	1.0893	1.0903	1.0903	1.0859	1.0883	1.0884	1.0884	1.0875	1.0876	1.0861	1.0861	1.0861
A(2,1,3)	111.3781	111.2407	110.5037	110.9022	110.6328	110.941	110.9427	110.948	110.8887	110.9033	110.9164	110.9497	110.952
A(2,1,4)	109.903	109.6825	109.3513	109.6105	109.6273	109.6896	109.6691	109.6767	109.6709	109.6608	109.6943	109.7119	109.7148
A(2,1,5)	109.6025	110.2333	110.7856	110.2281	110.609	110.5892	110.6179	110.6102	110.596	110.6208	110.5642	110.5503	110.5481
A(3,1,4)	110.2537	109.8513	109.5728	109.9337	109.7419	109.8335	109.8182	109.8226	109.838	109.8279	109.8507	109.867	109.87
A(3,1,5)	108.5005	109.3139	110.1805	109.3533	109.8405	109.8023	109.8265	109.8095	109.7997	109.8109	109.7739	109.7509	109.7465
A(4,1,5)	107.0948	106.4007	106.3529	106.723	106.2946	105.8602	105.8401	105.8477	105.9281	105.8953	105.9204	105.8873	105.8854
A(1,5,6)	95.0849	100.4221	100.7756	100.5971	99.957	101.2665	101.3046	101.3055	101.3613	101.4179	101.4206	101.4315	101.4358
A(5,6,7)	95.0818	100.4253	100.7748	100.6022	99.9592	101.2641	101.3026	101.3035	101.3589	101.4156	101.4187	101.4297	101.434
A(6,7,8)	107.0963	106.3986	106.3538	106.7111	106.2929	105.8619	105.8415	105.8491	105.9298	105.8969	105.9217	105.8885	105.8866
A(6,7,9)	109.5991	110.236	110.7837	110.2341	110.606	110.5885	110.617	110.6094	110.5957	110.6203	110.5635	110.5494	110.5473
A(6,7,10)	108.4976	109.3173	110.1805	109.3609	109.8444	109.7999	109.8247	109.8077	109.7969	109.8085	109.7722	109.7496	109.7451
A(8,7,9)	109.9045	109.681	109.3505	109.6072	109.6247	109.6902	109.6696	109.6772	109.6716	109.6614	109.6946	109.7122	109.7151
A(8,7,10)	110.2559	109.8496	109.574	109.9321	109.7448	109.834	109.8188	109.8231	109.8383	109.8282	109.8512	109.8674	109.8704
A(9,7,10)	111.379	111.24	110.5044	110.9049	110.6331	110.9414	110.9431	110.9484	110.8891	110.9038	110.9168	110.9501	110.9524
D(2,1,5,6)	-66.6663	-70.0423	-64.2448	-73.0268	-65.4057	-65.9201	-65.9803	-66.0116	-65.7322	-65.7874	-65.6151	-65.6171	-65.6541
D(3,1,5,6)	55.15	52.5268	58.3482	49.1426	57.0002	56.8351	56.8127	56.7715	56.9599	56.9474	57.0731	57.0882	57.0498
D(4,1,5,6)	174.1506	171.0978	177.0211	168.0136	175.6596	175.3367	175.2974	175.2568	175.5036	175.4664	175.6142	175.6179	175.5797
D(1,5,6,7)	85.3231	87.0756	88.5669	84.9414	87.7186	88.3644	88.3925	88.3419	88.3361	88.5283	88.5511	88.5314	88.5293
D(5,6,7,8)	174.1556	171.1182	177.0373	168.148	175.7416	175.3083	175.2753	175.2344	175.4686	175.435	175.5899	175.597	175.5576
D(5,6,7,9)	-66.6605	-70.0235	-64.23	-72.9001	-65.3294	-65.9472	-66.0015	-66.0331	-65.7655	-65.8174	-65.6387	-65.6375	-65.6756
D(5,6,7,10)	55.153	52.5487	58.3624	49.2815	57.0776	56.8065	56.7903	56.7487	56.925	56.9159	57.0484	57.0669	57.0272
Energy	-4878.08280235	-4878.5507241	-4878.58639561	-4878.58870998	-4882.81974652	-4882.90178394	-4882.90269996	-4882.90284583	-4882.90612169	-4882.90704086	-4882.91727119	-4882.91782745	-4882.91788833
ZPE Correction	0.07687	0.075686	0.075775	0.075441	0.07598	0.075032	0.074998	0.074997	0.074912	0.074903	0.074997	0.074983	0.074979

S6d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.096	1.0959	1.0971	1.097	1.0928	1.0946	1.0948	1.0948	1.0937	1.0938	1.0923	1.0923	1.0923
R(1,3)	1.0952	1.0954	1.0966	1.0965	1.0921	1.0942	1.0944	1.0944	1.0933	1.0935	1.092	1.0919	1.0919
R(1,4)	1.0987	1.099	1.1002	1.0998	1.096	1.0982	1.0984	1.0984	1.0972	1.0973	1.0958	1.0958	1.0958
R(1,5)	2.0298	1.9979	1.9917	1.9989	2.0194	2.001	2.0011	2.0011	1.9933	1.9935	1.9923	1.9925	1.9926
R(5,6)	2.4378	2.3327	2.3368	2.334	2.4482	2.3604	2.3601	2.3601	2.3467	2.3467	2.3464	2.3465	2.3465
R(6,7)	2.0298	1.9978	1.9917	1.9989	2.0194	2.001	2.0011	2.0011	1.9933	1.9935	1.9923	1.9925	1.9926
R(7,8)	1.0987	1.099	1.1002	1.0998	1.096	1.0982	1.0984	1.0984	1.0972	1.0973	1.0958	1.0958	1.0958
R(7,9)	1.0959	1.0959	1.0971	1.097	1.0928	1.0946	1.0948	1.0948	1.0937	1.0938	1.0923	1.0923	1.0923
R(7,10)	1.0952	1.0954	1.0966	1.0965	1.0921	1.0942	1.0944	1.0944	1.0933	1.0935	1.092	1.0919	1.0919
A(2,1,3)	111.6227	111.3145	110.5999	111.1251	110.8564	111.0116	111.0353	111.0384	110.9537	110.9934	110.9788	111.0271	111.0299
A(2,1,4)	110.45	110.0984	109.7384	110.0512	110.0542	110.0501	110.0359	110.0431	110.0303	110.0302	110.0411	110.0653	110.0688
A(2,1,5)	108.7877	109.6153	110.0856	109.4826	109.8485	109.9081	109.94	109.9326	109.8952	109.9327	109.8927	109.852	109.855
A(3,1,4)	110.9398	110.359	110.0808	110.4869	110.3037	110.3057	110.2919	110.2962	110.3071	110.2998	110.3066	110.336	110.338
A(3,1,5)	107.7177	108.6779	109.7352	108.6287	109.3217	109.382	109.3921	109.3755	109.417	109.3996	109.406	109.3752	109.3667
A(4,1,5)	107.1566	106.6518	106.5182	106.9599	106.3523	106.0615	106.0214	106.0308	106.1213	106.065	106.0971	106.062	106.0588
A(1,5,6)	94.5077	99.9411	100.1692	100.0459	99.1047	100.6958	100.7418	100.7411	100.7758	100.8627	100.867	100.8485	100.8557
A(5,6,7)	94.5069	99.9427	100.1738	100.0441	99.1071	100.6953	100.7413	100.7407	100.7756	100.8626	100.8668	100.8483	100.8555
A(6,7,8)	107.154	106.6506	106.5157	106.9616	106.3512	106.0622	106.022	106.0314	106.1218	106.0653	106.0975	106.0625	106.0592
A(6,7,9)	108.7866	109.6179	110.0809	109.4808	109.8462	109.9069	109.939	109.9316	109.894	109.9317	109.8914	109.8509	109.8539
A(6,7,10)	107.7185	108.6808	109.7422	108.6261	109.3253	109.382	109.3921	109.3756	109.4172	109.3999	109.4061	109.3752	109.3668
A(8,7,9)	110.451	110.0969	109.7353	110.0519	110.053	110.0503	110.036	110.0432	110.0305	110.0302	110.0412	110.0655	110.0689
A(8,7,10)	110.9394	110.3573	110.083	110.4881	110.3048	110.3061	110.2922	110.2965	110.3075	110.3001	110.3071	110.3365	110.3384
A(9,7,10)	111.6248	111.3133	110.6008	111.1259	110.8563	111.0116	111.0352	111.0383	110.9537	110.9933	110.9789	111.0271	111.0299
D(2,1,5,6)	-67.8644	-70.8673	-62.1	-74.2719	-62.7735	-63.8296	-64.0326	-64.0873	-63.429	-63.7468	-63.4826	-63.2776	-63.3878
D(3,1,5,6)	53.2867	50.9902	59.8502	47.2408	59.0748	58.2883	58.1418	58.0755	58.6314	58.3757	58.6002	58.8191	58.7089
D(4,1,5,6)	172.7118	169.9652	178.9846	166.5117	178.1583	177.2423	177.0623	176.9976	177.639	177.3339	177.5879	177.8057	177.6917
D(1,5,6,7)	82.6815	84.7563	85.781	82.3845	84.8311	85.9112	85.8874	85.822	85.7798	86.0543	86.015	85.8718	85.8805
D(5,6,7,8)	172.7889	169.9696	179.0859	166.4896	178.2221	177.2547	177.0727	177.0083	177.6541	177.3472	177.6018	177.8171	177.7032
D(5,6,7,9)	-67.7882	-70.8639	-62.0065	-74.2933	-62.713	-63.8173	-64.0222	-64.0767	-63.4142	-63.7337	-63.4689	-63.2663	-63.3764
D(5,6,7,10)	53.3652	50.9957	59.9463	47.2177	59.1359	58.2998	58.1515	58.0854	58.6455	58.3883	58.6132	58.8297	58.7197
Energy	-4880.51383016	-4880.9658851	-4881.00301537	-4881.00555008	-4885.22011717	-4885.29757942	-4885.29879005	-4885.29888672	-4885.30211755	-4885.30338356	-4885.3114877	-4885.31226239	-4885.31231458
ZPE Correction	0.074295	0.073239	0.073271	0.073006	0.073441	0.07252	0.072477	0.07247	0.072424	0.072409	0.072501	0.072494	0.072489

S6e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.091	1.0911	1.0923	1.0922	1.0875	1.0899	1.09	1.0899	1.089	1.0891	1.0875	1.0875	1.0875
R(1,3)	1.0903	1.0907	1.0919	1.0918	1.0871	1.0895	1.0897	1.0897	1.0887	1.0888	1.0873	1.0872	1.0872
R(1,4)	1.0937	1.0944	1.0956	1.0952	1.0909	1.0936	1.0937	1.0937	1.0926	1.0928	1.0912	1.0912	1.0912
R(1,5)	1.9981	1.972	1.9665	1.9721	1.99	1.9754	1.9753	1.9754	1.9685	1.9685	1.9682	1.9684	1.9684
R(5,6)	2.4207	2.3199	2.3227	2.3204	2.4244	2.3419	2.3417	2.3417	2.3285	2.3286	2.329	2.3291	2.3291
R(6,7)	1.9982	1.9719	1.9665	1.9721	1.99	1.9754	1.9753	1.9754	1.9685	1.9685	1.9682	1.9684	1.9684
R(7,8)	1.0937	1.0944	1.0956	1.0952	1.0909	1.0936	1.0937	1.0937	1.0926	1.0928	1.0912	1.0912	1.0912
R(7,9)	1.091	1.0911	1.0923	1.0922	1.0875	1.0898	1.09	1.0899	1.089	1.0891	1.0875	1.0875	1.0875
R(7,10)	1.0903	1.0907	1.0919	1.0918	1.0871	1.0895	1.0897	1.0896	1.0887	1.0888	1.0873	1.0872	1.0872
A(2,1,3)	111.4536	111.2844	110.578	111.0038	110.7085	110.9846	110.9992	111.0017	110.9432	110.9686	110.9725	111.0106	111.0115
A(2,1,4)	110.0424	109.8114	109.4852	109.7368	109.7458	109.8108	109.7892	109.7976	109.7985	109.7894	109.8154	109.8322	109.8351
A(2,1,5)	109.3757	110.0088	110.5322	109.9691	110.3769	110.3475	110.3719	110.3609	110.3508	110.3741	110.3307	110.3129	110.311
A(3,1,4)	110.4624	110.0426	109.7662	110.1369	109.9272	110.0099	109.9954	110.0012	110.0148	110.0068	110.0244	110.0412	110.0441
A(3,1,5)	108.2868	109.1419	110.0063	109.1383	109.6831	109.6498	109.6728	109.6567	109.6525	109.6591	109.6363	109.6144	109.6096
A(4,1,5)	107.0991	106.4313	106.3829	106.7614	106.3041	105.915	105.8872	105.8979	105.9619	105.9206	105.9401	105.9046	105.9046
A(1,5,6)	94.7538	100.0251	100.3723	100.2221	99.6109	100.895	100.9365	100.9333	101.0166	101.0832	101.0913	101.1056	101.1063
A(5,6,7)	94.7543	100.0286	100.3746	100.2264	99.6133	100.8971	100.9385	100.9351	101.0185	101.0847	101.0933	101.1078	101.1084
A(6,7,8)	107.0971	106.4285	106.382	106.7545	106.3029	105.9136	105.8859	105.8967	105.9606	105.9196	105.9388	105.9033	105.9033
A(6,7,9)	109.3757	110.0122	110.5297	109.9735	110.3757	110.3431	110.3679	110.3569	110.3458	110.3698	110.3257	110.3078	110.3061
A(6,7,10)	108.2865	109.1457	110.0094	109.1432	109.6858	109.6553	109.6779	109.6617	109.6584	109.664	109.6422	109.6205	109.6154
A(8,7,9)	110.0426	109.8097	109.4828	109.7349	109.7446	109.8088	109.7872	109.7957	109.7966	109.7877	109.8134	109.8301	109.833
A(8,7,10)	110.4628	110.0404	109.7682	110.1354	109.9282	110.0116	109.997	110.0028	110.0165	110.0084	110.0263	110.0432	110.046
A(9,7,10)	111.4551	111.2839	110.5788	111.0046	110.7083	110.9852	110.9997	111.0023	110.9438	110.9691	110.973	111.011	111.0119
D(2,1,5,6)	-66.8631	-69.1094	-63.3013	-73.0411	-64.4042	-64.9822	-65.0178	-65.0172	-64.8288	-64.8744	-64.7116	-64.6631	-64.6973
D(3,1,5,6)	54.7744	53.2561	59.0963	48.9485	57.8379	57.5646	57.5787	57.5645	57.67	57.6761	57.7998	57.8697	57.8323
D(4,1,5,6)	173.9095	171.9799	177.9237	167.9672	176.6393	176.2263	176.2195	176.2098	176.3653	176.3422	176.4857	176.5442	176.5076
D(1,5,6,7)	84.3953	86.3794	87.7191	83.944	86.7554	87.657	87.6179	87.5655	87.6405	87.8338	87.9015	87.8583	87.8552
D(5,6,7,8)	173.9506	172.0013	177.984	168.0482	176.6903	176.2995	176.287	176.2753	176.438	176.4015	176.557	176.6186	176.5789
D(5,6,7,9)	-66.823	-69.09	-63.2458	-72.964	-64.3559	-64.9145	-64.9556	-64.9569	-64.7618	-64.8199	-64.6462	-64.5947	-64.6318
D(5,6,7,10)	54.8162	53.2797	59.1531	49.0326	57.8869	57.6337	57.6423	57.6261	57.7383	57.7316	57.8665	57.9394	57.899
Energy	-4877.77501011	-4878.24035025	-4878.27688389	-4878.27927733	-4882.52084409	-4882.60221704	-4882.60322265	-4882.60332889	-4882.60634068	-4882.60735756	-4882.61735701	-4882.61799782	-4882.61804776
ZPE Correction	0.076535	0.075341	0.075487	0.075143	0.075695	0.074773	0.074736	0.074734	0.07468	0.074666	0.074742	0.074731	0.07473

S6f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.09	1.0903	1.0914	1.0914	1.0865	1.0891	1.0893	1.0893	1.0885	1.0887	1.0877	1.0876	1.0876
R(1,3)	1.0892	1.0897	1.0911	1.0908	1.0861	1.0887	1.089	1.089	1.0881	1.0884	1.0874	1.0874	1.0873
R(1,4)	1.093	1.0935	1.0948	1.0945	1.0901	1.0929	1.0931	1.0931	1.0921	1.0924	1.0913	1.0913	1.0913
R(1,5)	1.9943	1.9636	1.9582	1.9636	1.988	1.97	1.9702	1.9702	1.9629	1.9633	1.9621	1.9623	1.9624
R(5,6)	2.4197	2.3069	2.3101	2.3078	2.4313	2.3369	2.3371	2.3371	2.3226	2.3231	2.322	2.3226	2.3226
R(6,7)	1.9943	1.9636	1.9582	1.9636	1.988	1.9701	1.9702	1.9702	1.9629	1.9633	1.9621	1.9623	1.9624
R(7,8)	1.093	1.0935	1.0948	1.0945	1.0901	1.0929	1.0931	1.0931	1.0921	1.0924	1.0913	1.0913	1.0913
R(7,9)	1.09	1.0903	1.0914	1.0914	1.0865	1.0891	1.0893	1.0893	1.0885	1.0887	1.0877	1.0876	1.0876
R(7,10)	1.0892	1.0897	1.0911	1.0908	1.0861	1.0887	1.089	1.089	1.0881	1.0884	1.0874	1.0873	1.0873
A(2,1,3)	111.4366	111.1426	110.4081	110.8431	110.7252	110.8817	110.9273	110.925	110.8317	110.8848	110.833	110.8863	110.8859
A(2,1,4)	109.9046	109.5592	109.245	109.489	109.651	109.6467	109.6283	109.6304	109.6226	109.6253	109.6195	109.6322	109.6344
A(2,1,5)	109.6683	110.3797	110.9949	110.423	110.7059	110.7182	110.7376	110.728	110.749	110.7492	110.7773	110.752	110.749
A(3,1,4)	110.2494	109.7539	109.4615	109.8007	109.7474	109.8018	109.7867	109.7904	109.7922	109.7992	109.7753	109.7906	109.7939
A(3,1,5)	108.7227	109.6465	110.4678	109.716	109.9831	110.0206	110.033	110.0272	110.0463	110.0289	110.0541	110.0313	110.0257
A(4,1,5)	106.7372	106.2382	106.1598	106.4716	105.9148	105.6399	105.5908	105.6035	105.6705	105.62	105.6519	105.6146	105.6186
A(1,5,6)	95.992	101.2452	101.7237	101.5109	101.0885	102.1947	102.2426	102.2376	102.2992	102.3571	102.3905	102.4048	102.3951
A(5,6,7)	95.9904	101.2498	101.7224	101.5119	101.0876	102.1926	102.2409	102.2359	102.2965	102.3552	102.3881	102.4028	102.3932
A(6,7,8)	106.7375	106.2332	106.161	106.4671	105.9148	105.6413	105.592	105.6046	105.6725	105.6215	105.6537	105.616	105.62
A(6,7,9)	109.666	110.3818	110.9932	110.4248	110.7049	110.7165	110.7361	110.7265	110.7478	110.7479	110.7761	110.7507	110.7477
A(6,7,10)	108.7208	109.6548	110.4668	109.7176	109.9818	110.0184	110.0313	110.0256	110.0431	110.0268	110.0512	110.0293	110.0236
A(8,7,9)	109.9055	109.5562	109.245	109.4884	109.6517	109.6475	109.6289	109.631	109.6237	109.6261	109.6205	109.6329	109.6351
A(8,7,10)	110.251	109.7524	109.4626	109.8009	109.7483	109.8025	109.7874	109.7911	109.7927	109.7997	109.7758	109.7912	109.7944
A(9,7,10)	111.4379	111.1416	110.4087	110.8444	110.7259	110.8825	110.9281	110.9257	110.8326	110.8855	110.8338	110.887	110.8865
D(2,1,5,6)	-65.8657	-70.0812	-64.5967	-72.1954	-66.2686	-66.2806	-66.28	-66.2428	-66.134	-66.004	-66.2199	-66.0286	-66.0449
D(3,1,5,6)	56.2033	52.683	58.2168	50.2679	56.4156	56.6355	56.7158	56.7395	56.7574	56.9429	56.6979	56.9238	56.9011
D(4,1,5,6)	175.1198	171.2222	176.7982	169.0321	174.9402	175.0879	175.129	175.1612	175.2291	175.3853	175.143	175.3542	175.3346
D(1,5,6,7)	84.8348	86.3792	88.3179	84.9499	87.3633	87.8207	87.6815	87.6357	87.8127	87.9133	87.9249	87.8567	87.8267
D(5,6,7,8)	175.1185	171.3247	176.8013	169.073	174.929	175.0648	175.1106	175.1434	175.1951	175.3602	175.1122	175.3304	175.3114
D(5,6,7,9)	-65.8671	-69.984	-64.5938	-72.1569	-66.2796	-66.3028	-66.2977	-66.26	-66.1662	-66.0281	-66.2491	-66.0514	-66.0671
D(5,6,7,10)	56.201	52.7858	58.2184	50.3103	56.4041	56.6119	56.6969	56.7211	56.7234	56.9175	56.6669	56.8996	56.8774
Energy	-4880.73818507	-4881.19553229	-4881.23387219	-4881.23620029	-4885.44391348	-4885.5254422	-4885.52717659	-4885.52723647	-4885.52871614	-4885.53051987	-4885.53906675	-4885.54009563	-4885.54016028
ZPE Correction	0.076078	0.074955	0.074931	0.074658	0.075276	0.074292	0.074225	0.074214	0.07409	0.074056	0.074104	0.074096	0.074098

S6g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.089	1.0894	1.0905	1.0906	1.0859	1.0884	1.0886	1.0887	1.0877	1.0879	1.0868	1.0868	1.0868
R(1,3)	1.0885	1.089	1.0902	1.09	1.0856	1.0881	1.0884	1.0884	1.0875	1.0877	1.0866	1.0866	1.0866
R(1,4)	1.0923	1.0929	1.0941	1.0938	1.0895	1.0923	1.0926	1.0926	1.0916	1.0918	1.0906	1.0907	1.0907
R(1,5)	1.9919	1.9637	1.9584	1.9635	1.9852	1.9689	1.969	1.9691	1.9621	1.9623	1.9615	1.9617	1.9618
R(5,6)	2.4158	2.3075	2.3098	2.3077	2.4206	2.3327	2.3326	2.3326	2.3194	2.3196	2.3192	2.3195	2.3195
R(6,7)	1.9919	1.9637	1.9584	1.9635	1.9852	1.9689	1.969	1.9691	1.9621	1.9623	1.9615	1.9618	1.9618
R(7,8)	1.0922	1.0929	1.0941	1.0938	1.0895	1.0923	1.0926	1.0926	1.0916	1.0918	1.0906	1.0907	1.0907
R(7,9)	1.089	1.0894	1.0905	1.0905	1.0859	1.0884	1.0886	1.0887	1.0877	1.0879	1.0868	1.0868	1.0868
R(7,10)	1.0884	1.089	1.0902	1.09	1.0856	1.0881	1.0884	1.0884	1.0875	1.0877	1.0866	1.0866	1.0866
A(2,1,3)	111.4369	111.2065	110.4956	110.8774	110.7114	110.9284	110.9587	110.9579	110.8877	110.9289	110.8893	110.942	110.9429
A(2,1,4)	109.9241	109.6088	109.307	109.5446	109.644	109.6589	109.6436	109.6465	109.6455	109.6468	109.638	109.66	109.6624
A(2,1,5)	109.6876	110.3676	110.958	110.4031	110.7133	110.7167	110.7444	110.7372	110.7292	110.7403	110.7556	110.728	110.7262
A(3,1,4)	110.2152	109.775	109.4973	109.8401	109.7393	109.8048	109.7921	109.7951	109.8062	109.811	109.7874	109.8103	109.8131
A(3,1,5)	108.6869	109.5743	110.37	109.6403	109.9671	109.986	110.0004	109.9921	109.988	109.9792	110.0017	109.9688	109.964
A(4,1,5)	106.7691	106.1827	106.1062	106.4357	105.9544	105.6105	105.5616	105.5726	105.6524	105.5982	105.6357	105.5945	105.5953
A(1,5,6)	95.8749	101.1263	101.6102	101.3994	100.9435	102.0685	102.1211	102.1163	102.1428	102.2103	102.2454	102.2637	102.2595
A(5,6,7)	95.8706	101.1281	101.608	101.4001	100.9429	102.0664	102.1193	102.1146	102.1401	102.2083	102.2429	102.2617	102.2575
A(6,7,8)	106.7714	106.1814	106.1079	106.4299	105.9543	105.6122	105.563	105.5739	105.6547	105.5999	105.6378	105.5962	105.5969
A(6,7,9)	109.6825	110.3695	110.9568	110.4057	110.7121	110.7152	110.743	110.7358	110.7284	110.7391	110.7546	110.7268	110.7249
A(6,7,10)	108.6835	109.5764	110.3682	109.6421	109.9666	109.9841	109.9991	109.9909	109.985	109.9774	109.9992	109.9672	109.9624
A(8,7,9)	109.926	109.6079	109.3074	109.5435	109.6442	109.6594	109.644	109.6469	109.6464	109.6474	109.6387	109.6605	109.6628
A(8,7,10)	110.2184	109.7739	109.4978	109.8402	109.7402	109.8054	109.7927	109.7957	109.8065	109.8114	109.7878	109.8108	109.8135
A(9,7,10)	111.4379	111.2058	110.4961	110.8795	110.712	110.9289	110.9592	110.9583	110.8882	110.9294	110.8897	110.9425	110.9433
D(2,1,5,6)	-65.9595	-69.7314	-64.7959	-72.4291	-66.1769	-66.1942	-66.2588	-66.2521	-66.0215	-65.9869	-66.0693	-65.9964	-66.0182
D(3,1,5,6)	56.0993	53.0566	58.0355	50.0135	56.484	56.7564	56.759	56.7541	56.8875	56.9757	56.869	56.9673	56.9421
D(4,1,5,6)	174.974	171.5517	176.5764	168.7636	175.0131	175.1778	175.1454	175.1459	175.3353	175.3942	175.2923	175.3775	175.3534
D(1,5,6,7)	85.7993	87.3338	88.9926	85.6139	88.0372	88.4813	88.39	88.3416	88.4857	88.5942	88.6404	88.5594	88.5519
D(5,6,7,8)	174.9721	171.5624	176.5628	168.8202	175.0082	175.1591	175.1323	175.1334	175.3041	175.3746	175.2654	175.36	175.3364
D(5,6,7,9)	-65.9606	-69.7214	-64.8086	-72.3758	-66.1821	-66.212	-66.2713	-66.2641	-66.0508	-66.0055	-66.0947	-66.0131	-66.0345
D(5,6,7,10)	56.0942	53.0683	58.0213	50.0723	56.4784	56.737	56.7452	56.7408	56.8562	56.9557	56.8417	56.9492	56.9244
Energy	-4879.07463681	-4879.53677227	-4879.57464664	-4879.57692688	-4883.80540799	-4883.88803004	-4883.88973502	-4883.88982006	-4883.89131494	-4883.8931156	-4883.90224931	-4883.90327659	-4883.90333108
ZPE Correction	0.076651	0.075521	0.075582	0.075234	0.075871	0.074911	0.074845	0.074832	0.074732	0.074702	0.074756	0.074741	0.074739

S6h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0974	1.0971	1.0985	1.0984	1.0938	1.0958	1.0959	1.0959	1.095	1.0951	1.0937	1.0936	1.0937
R(1,3)	1.0966	1.0968	1.0981	1.098	1.0935	1.0955	1.0957	1.0957	1.0947	1.0949	1.0935	1.0935	1.0935
R(1,4)	1.1003	1.1006	1.102	1.1016	1.0976	1.0998	1.1	1.1	1.0988	1.099	1.0976	1.0976	1.0976
R(1,5)	2.0045	1.9774	1.9716	1.9778	1.9982	1.9819	1.9818	1.9819	1.9743	1.9744	1.9738	1.9739	1.974
R(5,6)	2.428	2.3205	2.3241	2.3215	2.4342	2.346	2.3458	2.3458	2.3331	2.3333	2.3329	2.3331	2.3331
R(6,7)	2.0046	1.9774	1.9716	1.9778	1.9982	1.9819	1.9818	1.9819	1.9743	1.9745	1.9738	1.9739	1.974
R(7,8)	1.1003	1.1006	1.102	1.1016	1.0976	1.0998	1.1	1.1	1.0988	1.099	1.0976	1.0976	1.0976
R(7,9)	1.0974	1.0971	1.0985	1.0984	1.0938	1.0958	1.0959	1.0959	1.095	1.0951	1.0937	1.0936	1.0937
R(7,10)	1.0966	1.0968	1.0981	1.098	1.0935	1.0955	1.0957	1.0957	1.0947	1.0949	1.0935	1.0935	1.0935
A(2,1,3)	111.5186	111.3588	110.6177	111.067	110.8111	111.0686	111.0903	111.0924	111.0365	111.0735	111.0656	111.116	111.1167
A(2,1,4)	110.0369	109.8268	109.4377	109.7439	109.7365	109.8095	109.7827	109.791	109.8134	109.8047	109.826	109.8471	109.85
A(2,1,5)	109.3934	110.0542	110.6642	110.0082	110.4788	110.4622	110.4988	110.4882	110.441	110.4672	110.4353	110.4089	110.4067
A(3,1,4)	110.4645	110.0142	109.6869	110.0876	109.8745	109.9618	109.9404	109.9459	109.9899	109.9808	109.9906	110.0122	110.0157
A(3,1,5)	108.2394	109.0585	110.0805	109.1195	109.71	109.6433	109.6711	109.6542	109.6189	109.6272	109.6119	109.5846	109.5796
A(4,1,5)	107.0625	106.4025	106.2554	106.7157	106.1226	105.7609	105.7199	105.7321	105.8107	105.7524	105.7781	105.7339	105.734
A(1,5,6)	94.786	100.4071	100.8216	100.5973	100.018	101.3751	101.4299	101.4279	101.4064	101.4899	101.5076	101.5147	101.5143
A(5,6,7)	94.7848	100.4094	100.8279	100.5938	100.022	101.3725	101.4277	101.4257	101.403	101.4869	101.5041	101.5118	101.5113
A(6,7,8)	107.0611	106.4013	106.2518	106.7181	106.121	105.7623	105.7211	105.7333	105.8128	105.7542	105.7803	105.7356	105.7358
A(6,7,9)	109.391	110.0563	110.6595	110.0047	110.4766	110.46	110.4968	110.4862	110.4396	110.4657	110.4341	110.4074	110.4052
A(6,7,10)	108.238	109.0609	110.0888	109.1165	109.7147	109.6418	109.67	109.6529	109.616	109.6248	109.6087	109.5824	109.5774
A(8,7,9)	110.0377	109.8259	109.4328	109.7446	109.7345	109.8103	109.7833	109.7917	109.8145	109.8056	109.8272	109.8479	109.8509
A(8,7,10)	110.4666	110.0127	109.6902	110.0896	109.8757	109.9626	109.9411	109.9466	109.9904	109.9814	109.991	110.0128	110.0163
A(9,7,10)	111.5206	111.3579	110.6191	111.0685	110.811	111.0694	111.091	111.093	111.0371	111.0741	111.0661	111.1166	111.1173
D(2,1,5,6)	-67.2665	-71.2819	-63.9901	-73.9036	-65.2835	-66.3146	-66.3939	-66.4246	-66.0667	-66.0837	-66.004	-65.8825	-65.923
D(3,1,5,6)	54.4318	51.151	58.5965	48.1772	57.1725	56.4092	56.4003	56.3536	56.5862	56.6387	56.677	56.8261	56.7817
D(4,1,5,6)	173.524	169.7814	177.2956	167.1015	175.8225	174.9243	174.8814	174.8393	175.1497	175.1632	175.2194	175.3553	175.3125
D(1,5,6,7)	84.272	86.2089	87.9777	84.1999	87.0345	87.7933	87.7713	87.7065	87.7979	87.9988	88.0387	87.9881	87.976
D(5,6,7,8)	173.5655	169.7923	177.4143	167.0723	175.9028	174.8884	174.8484	174.8047	175.0954	175.1151	175.161	175.3096	175.2666
D(5,6,7,9)	-67.2261	-71.2717	-63.882	-73.9325	-65.2078	-66.3499	-66.4265	-66.4587	-66.1193	-66.1304	-66.0604	-65.927	-65.9676
D(5,6,7,10)	54.4724	51.163	58.709	48.146	57.2497	56.3724	56.3664	56.3182	56.5316	56.5902	56.6184	56.7799	56.7353
Energy	-4877.25465168	-4877.72398707	-4877.76165957	-4877.76410821	-4881.98136088	-4882.06351181	-4882.06483369	-4882.06493281	-4882.0674588	-4882.06883138	-4882.07801092	-4882.07885733	-4882.07891122
ZPE Correction	0.074763	0.073581	0.073545	0.073289	0.073808	0.072857	0.072808	0.072802	0.072737	0.072722	0.072821	0.072802	0.072801

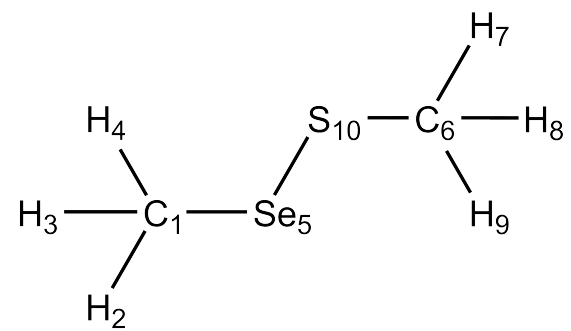
S6i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0915	1.0916	1.0927	1.0927	1.0879	1.0901	1.0902	1.0902	1.0892	1.0892	1.0876	1.0875	1.0875
R(1,3)	1.0909	1.0912	1.0923	1.0923	1.0875	1.0898	1.0899	1.0899	1.0889	1.089	1.0874	1.0873	1.0873
R(1,4)	1.0943	1.095	1.0961	1.0957	1.0914	1.0939	1.094	1.094	1.0928	1.093	1.0913	1.0913	1.0913
R(1,5)	1.9973	1.9704	1.9648	1.9705	1.9887	1.9734	1.9733	1.9733	1.9665	1.9665	1.9661	1.9662	1.9663
R(5,6)	2.4174	2.3168	2.3198	2.3174	2.4232	2.3398	2.3395	2.3396	2.3258	2.3259	2.3263	2.3263	2.3263
R(6,7)	1.9973	1.9703	1.9648	1.9705	1.9887	1.9734	1.9733	1.9733	1.9665	1.9665	1.9661	1.9662	1.9663
R(7,8)	1.0943	1.095	1.0961	1.0957	1.0914	1.0939	1.094	1.094	1.0928	1.093	1.0913	1.0913	1.0913
R(7,9)	1.0915	1.0916	1.0927	1.0927	1.0879	1.0901	1.0902	1.0902	1.0892	1.0892	1.0876	1.0875	1.0875
R(7,10)	1.0909	1.0912	1.0923	1.0923	1.0875	1.0898	1.0899	1.0899	1.0889	1.089	1.0874	1.0873	1.0873
A(2,1,3)	111.4786	111.3113	110.5939	111.0039	110.7572	111.0324	111.0396	111.044	110.9873	111.0067	111.0164	111.0546	111.057
A(2,1,4)	110.0474	109.8083	109.4777	109.7375	109.7548	109.818	109.7969	109.8053	109.8022	109.7926	109.8201	109.8391	109.8422
A(2,1,5)	109.4386	110.0632	110.6037	110.0288	110.4287	110.4058	110.434	110.4247	110.4007	110.4252	110.375	110.3563	110.3543
A(3,1,4)	110.4229	110.0156	109.7333	110.105	109.9054	109.9886	109.9741	109.9793	109.9975	109.9887	110.009	110.0276	110.0306
A(3,1,5)	108.3284	109.1597	110.0496	109.179	109.7011	109.6635	109.6854	109.6687	109.6622	109.67	109.6446	109.618	109.6127
A(4,1,5)	107.0009	106.3583	106.2877	106.6899	106.1918	105.8022	105.779	105.787	105.8657	105.8298	105.8482	105.8143	105.8127
A(1,5,6)	94.989	100.2359	100.5797	100.4206	99.8322	101.1231	101.1632	101.1637	101.2228	101.2826	101.2772	101.2824	101.2859
A(5,6,7)	94.9882	100.2413	100.5815	100.423	99.8343	101.1231	101.1632	101.1637	101.2212	101.2811	101.2764	101.2818	101.2851
A(6,7,8)	106.9998	106.3543	106.2869	106.6854	106.1907	105.8019	105.7787	105.7867	105.8664	105.8306	105.8484	105.8143	105.8129
A(6,7,9)	109.4372	110.0676	110.6011	110.0316	110.4276	110.4036	110.4319	110.4227	110.3999	110.4244	110.3736	110.3548	110.3529
A(6,7,10)	108.3271	109.1644	110.0524	109.1818	109.7035	109.665	109.687	109.6702	109.6612	109.669	109.6449	109.6187	109.6131
A(8,7,9)	110.0481	109.8061	109.4752	109.7362	109.7538	109.8173	109.7961	109.8046	109.802	109.7925	109.8195	109.8384	109.8416
A(8,7,10)	110.4242	110.0128	109.7353	110.1045	109.9064	109.9895	109.9749	109.9801	109.9979	109.989	110.0097	110.0283	110.0313
A(9,7,10)	111.4801	111.311	110.5949	111.0044	110.757	111.033	111.0402	111.0446	110.9881	111.0074	111.0172	111.0554	111.0578
D(2,1,5,6)	-66.7994	-69.7676	-63.5929	-73.1926	-64.8217	-65.4315	-65.5185	-65.5404	-65.1866	-65.2591	-65.0202	-64.9981	-65.0434
D(3,1,5,6)	54.9325	52.678	58.902	48.8616	57.5276	57.2228	57.1784	57.1447	57.4069	57.3803	57.581	57.6209	57.5739
D(4,1,5,6)	173.9894	171.3385	177.6584	167.824	176.2489	175.803	175.7398	175.7082	176.0326	175.9795	176.2014	176.2304	176.1834
D(1,5,6,7)	85.1039	86.6718	88.1457	84.389	87.1897	88.0064	88.0097	87.953	88.0158	88.2006	88.2388	88.1969	88.1897
D(5,6,7,8)	174.0106	171.3631	177.7142	167.8661	176.2955	175.8164	175.7519	175.7193	176.0136	175.9591	176.1947	176.2284	176.1782
D(5,6,7,9)	-66.7786	-69.7455	-63.542	-73.1531	-64.7775	-65.4203	-65.5085	-65.5313	-65.2058	-65.2795	-65.0283	-65.0018	-65.0499
D(5,6,7,10)	54.9535	52.7056	58.9543	48.9054	57.5724	57.2345	57.1888	57.1542	57.3875	57.3596	57.5733	57.6177	57.5676
Energy	-4878.43945139	-4878.90382258	-4878.94003991	-4878.94241544	-4883.16846379	-4883.2480985	-4883.24905789	-4883.24918448	-4883.25297879	-4883.2539523	-4883.26360696	-4883.26420443	-4883.26425869
ZPE Correction	0.076171	0.074972	0.075119	0.074791	0.075304	0.074431	0.074396	0.074393	0.074352	0.074345	0.074422	0.074412	0.07441

S6j – QCISD

	QCISD/cc-pVTZ
R(1,2)	1.0860
R(1,3)	1.0854
R(1,4)	1.0890
R(1,5)	1.9513
R(5,6)	2.3182
R(6,7)	1.9513
R(7,8)	1.0890
R(7,9)	1.0860
R(7,10)	1.0854
A(2,1,3)	110.5993
A(2,1,4)	109.5758
A(2,1,5)	110.3322
A(3,1,4)	109.8977
A(3,1,5)	109.7738
A(4,1,5)	106.5801
A(1,5,6)	99.7527
A(5,6,7)	99.7533
A(6,7,8)	106.5801
A(6,7,9)	110.3301
A(6,7,10)	109.7759
A(8,7,9)	109.5751
A(8,7,10)	109.8986
A(9,7,10)	110.5993
D(2,1,5,6)	-63.1390
D(3,1,5,6)	58.9972
D(4,1,5,6)	177.9701
D(1,5,6,7)	86.0480
D(5,6,7,8)	177.9934
D(5,6,7,9)	-63.1178
D(5,6,7,10)	59.0184
Energies	-4879.8890184
ZPE Correction	0.07572

S7 – MeSeSMe



S7a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0891	1.0893	1.0905	1.0901	1.0852	1.0879	1.088	1.088	1.0868	1.0869	1.0852	1.0852	1.0852
R(1,3)	1.0884	1.0889	1.0902	1.0899	1.0847	1.0875	1.0877	1.0876	1.0865	1.0866	1.0849	1.0849	1.0849
R(1,4)	1.0929	1.0929	1.0939	1.0938	1.0888	1.0915	1.0917	1.0916	1.0903	1.0905	1.0887	1.0887	1.0887
R(1,5)	2.0029	1.9744	1.9704	1.9753	1.9934	1.9783	1.9785	1.9786	1.972	1.9721	1.9717	1.972	1.972
R(5,10)	2.3361	2.215	2.215	2.2139	2.3421	2.2301	2.2295	2.2295	2.2055	2.2051	2.2037	2.2034	2.2034
R(6,7)	1.0921	1.0938	1.0944	1.0944	1.0878	1.0925	1.0926	1.0926	1.0917	1.0919	1.0901	1.0902	1.0902
R(6,8)	1.0903	1.0913	1.0918	1.0917	1.085	1.0894	1.0895	1.0895	1.0884	1.0885	1.0869	1.0869	1.0869
R(6,9)	1.0894	1.0906	1.0913	1.0911	1.0845	1.0888	1.089	1.089	1.0879	1.0881	1.0864	1.0864	1.0864
R(6,10)	1.8974	1.8383	1.8373	1.8367	1.9011	1.8357	1.8357	1.8357	1.8285	1.8284	1.8241	1.8245	1.8245
A(2,1,3)	111.6072	111.4376	110.732	110.9662	110.7735	111.0642	111.0727	111.0899	110.9878	111.0045	111.0301	111.0573	111.057
A(2,1,4)	109.9712	109.7056	109.5039	109.6661	109.7851	109.761	109.7511	109.7547	109.7434	109.7415	109.7931	109.8138	109.8179
A(2,1,5)	109.8258	110.2745	110.7788	111.0941	110.4819	110.4165	110.4524	110.4551	110.4251	110.4515	110.3686	110.3361	110.3408
A(3,1,4)	110.217	109.9217	109.8594	110.0319	109.9532	110.0279	110.0143	110.018	110.0332	110.0296	110.0676	110.0969	110.0962
A(3,1,5)	108.8532	109.4209	109.7613	109.4965	109.5227	109.5302	109.5576	109.557	109.5488	109.5674	109.4958	109.4783	109.4748
A(4,1,5)	106.215	105.9322	106.0995	105.4434	106.223	105.9133	105.8627	105.8338	105.982	105.9225	105.962	105.9322	105.9276
A(1,5,10)	98.1279	100.8979	100.6865	100.719	99.1843	100.5643	100.7162	100.7337	101.0548	101.1793	101.0388	101.0953	101.1004
A(7,6,8)	110.0241	109.1921	109.0403	109.1968	110.0295	109.1558	109.1405	109.1421	109.1613	109.156	109.1221	109.1245	109.1249
A(7,6,9)	110.3973	109.5107	109.3334	109.4441	110.1596	109.366	109.3614	109.3584	109.4007	109.3996	109.3413	109.3621	109.364
A(7,6,10)	106.0151	106.1745	105.8968	106.1561	105.4025	105.7282	105.7372	105.7489	105.8728	105.8191	105.8405	105.7817	105.778
A(8,6,9)	110.8049	110.1345	110.1997	110.0731	111.0137	110.3761	110.3527	110.3736	110.3774	110.3826	110.3665	110.3913	110.3872
A(8,6,10)	110.0583	111.2696	111.3553	111.2354	110.3424	111.3265	111.3114	111.3051	111.2423	111.2478	111.3173	111.2993	111.2991
A(9,6,10)	109.4299	110.466	110.8958	110.641	109.748	110.7599	110.8099	110.7847	110.6664	110.7129	110.7285	110.7544	110.7602
A(5,10,6)	98.5155	102.5207	103.2897	102.4711	101.6527	103.3176	103.3851	103.3739	103.7204	103.7964	103.9423	103.9835	103.9897
D(2,1,5,10)	-62.0948	-64.6151	-65.7431	-59.6856	-65.2849	-64.8368	-65.107	-65.1015	-64.9195	-65.1019	-65.1342	-65.0826	-65.1632
D(3,1,5,10)	60.3674	58.2986	56.8476	63.2311	57.0008	57.7754	57.5578	57.5863	57.6148	57.4834	57.3807	57.4334	57.3532
D(4,1,5,10)	179.0266	176.7472	175.4936	-178.4225	175.7024	176.3954	176.1475	176.164	176.2892	176.1298	176.057	176.1184	176.0331
D(1,5,10,6)	85.677	87.1211	86.7375	88.7056	88.0413	87.4453	87.4102	87.4064	87.353	87.4653	87.3647	87.3791	87.3897
D(7,6,10,5)	175.3182	173.26	175.8923	178.7383	176.6274	176.1254	176.3747	176.4298	176.2284	176.2971	176.2506	176.3657	176.3661
D(8,6,10,5)	-65.7318	-68.0409	-65.7115	-62.5866	-64.6196	-65.456	-65.2276	-65.167	-65.3051	-65.2718	-65.309	-65.2357	-65.2372
D(9,6,10,5)	56.2568	54.6123	57.3901	60.0872	58.0259	57.7549	57.9781	58.0433	57.7814	57.8583	57.8606	57.9715	57.9688
Energy	-2877.14338654	-2877.41688611	-2877.43673567	-2877.43889221	-2879.54967063	-2879.62728138	-2879.62892228	-2879.62912558	-2879.63861442	-2879.64004869	-2879.64715694	-2879.64796406	-2879.648033
ZPE Correction	0.077098	0.076557	0.076447	0.07638	0.076536	0.076015	0.075931	0.075937	0.075932	0.07588	0.075998	0.075969	0.075965

S7b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0889	1.089	1.0902	1.0898	1.0856	1.0881	1.0882	1.0881	1.0872	1.0872	1.0857	1.0856	1.0856
R(1,3)	1.0881	1.0887	1.0899	1.0896	1.0851	1.0877	1.0879	1.0879	1.0869	1.087	1.0854	1.0854	1.0854
R(1,4)	1.0926	1.0926	1.0935	1.0934	1.089	1.0916	1.0917	1.0917	1.0906	1.0907	1.0891	1.0891	1.0891
R(1,5)	1.9827	1.9549	1.9504	1.9551	1.973	1.9589	1.959	1.9591	1.9531	1.9531	1.9527	1.9529	1.9529
R(5,10)	2.3139	2.1926	2.1926	2.1915	2.3166	2.2054	2.2052	2.2051	2.1817	2.1815	2.1801	2.18	2.18
R(6,7)	1.0916	1.0935	1.094	1.0939	1.088	1.0926	1.0927	1.0927	1.0919	1.092	1.0905	1.0905	1.0905
R(6,8)	1.0901	1.0911	1.0915	1.0913	1.0854	1.0895	1.0897	1.0896	1.0886	1.0887	1.0872	1.0873	1.0873
R(6,9)	1.0892	1.0905	1.091	1.0908	1.0849	1.089	1.0892	1.0892	1.0882	1.0883	1.0869	1.0869	1.0869
R(6,10)	1.8807	1.8232	1.8218	1.8212	1.8821	1.8199	1.8199	1.8199	1.8131	1.813	1.8089	1.8094	1.8094
A(2,1,3)	111.4769	111.4176	110.6324	110.853	110.5775	110.9963	110.9941	111.0152	110.9411	110.9446	110.9693	110.9868	110.9873
A(2,1,4)	109.7447	109.538	109.3219	109.4733	109.5646	109.5874	109.5715	109.5772	109.5909	109.5845	109.6426	109.6566	109.6625
A(2,1,5)	110.0437	110.446	110.9726	111.2897	110.7092	110.5898	110.6301	110.6318	110.5848	110.6158	110.5128	110.4893	110.4939
A(3,1,4)	110.0134	109.7466	109.6792	109.8531	109.7337	109.8551	109.8372	109.8417	109.8786	109.8713	109.9169	109.9405	109.9405
A(3,1,5)	109.0067	109.5142	109.873	109.6559	109.6919	109.6401	109.6692	109.6691	109.6261	109.6484	109.5617	109.5567	109.55
A(4,1,5)	106.4249	106.0344	106.261	105.5808	106.4771	106.052	106.0171	105.9816	106.1045	106.0592	106.1225	106.094	106.0896
A(1,5,10)	97.948	100.8659	100.583	100.6158	98.8815	100.438	100.5952	100.6136	100.9614	101.0715	100.9043	100.9607	100.9657
A(7,6,8)	109.836	109.048	108.8807	109.0391	109.8071	108.9881	108.9789	108.9823	109.0346	109.0302	109.0001	109.0027	109.0035
A(7,6,9)	110.2486	109.3819	109.1904	109.302	109.9459	109.2063	109.2114	109.2082	109.2806	109.2816	109.2228	109.2488	109.251
A(7,6,10)	106.2873	106.354	106.0553	106.3073	105.6582	105.8824	105.8965	105.9064	105.9851	105.9441	105.9534	105.9088	105.905
A(8,6,9)	110.6531	110.0526	110.1188	109.9965	110.817	110.2922	110.2668	110.293	110.345	110.3448	110.3377	110.3573	110.3518
A(8,6,10)	110.2012	111.4166	111.4851	111.3528	110.5531	111.4755	111.4475	111.4392	111.3537	111.35	111.4185	111.3912	111.3909
A(9,6,10)	109.5223	110.4952	110.9885	110.7467	109.935	110.8658	110.9104	110.8821	110.7194	110.7656	110.7809	110.8031	110.8097
A(5,10,6)	98.0441	102.3639	103.1451	102.3187	101.2863	103.1147	103.1925	103.1804	103.5386	103.6098	103.7654	103.7951	103.8036
D(2,1,5,10)	-61.7214	-64.9162	-66.1515	-59.8464	-65.2366	-64.9727	-65.3086	-65.2671	-65.1966	-65.4207	-65.3596	-65.322	-65.4238
D(3,1,5,10)	60.8177	58.1485	56.52	63.1693	57.0662	57.7428	57.4506	57.5198	57.4366	57.2526	57.2181	57.2588	57.1562
D(4,1,5,10)	179.4325	176.4957	175.1029	-178.5378	175.741	176.2936	175.9756	176.0302	176.0373	175.8308	175.8406	175.8906	175.7819
D(1,5,10,6)	85.2276	86.9236	86.4273	88.4533	87.8648	87.2443	87.2074	87.2153	87.1537	87.2913	87.1914	87.1969	87.2058
D(7,6,10,5)	175.3667	172.2948	175.5505	178.7348	176.7368	175.9026	176.1602	176.2122	175.9775	176.0366	176.0759	176.1627	176.1566
D(8,6,10,5)	-65.6734	-68.9906	-66.08	-62.6246	-64.5168	-65.7081	-65.468	-65.4105	-65.581	-65.5538	-65.5083	-65.4598	-65.4673
D(9,6,10,5)	56.2788	53.6804	57.0762	60.1078	58.1478	57.5766	57.7962	57.8612	57.5802	57.6376	57.7335	57.8037	57.7937
Energy	-2878.55450529	-2878.82901135	-2878.84715651	-2878.84926987	-2880.95978985	-2881.03950254	-2881.04119163	-2881.04144528	-2881.05158405	-2881.05298804	-2881.05996599	-2881.06069755	-2881.06077568
ZPE Correction	0.077545	0.076845	0.076783	0.076723	0.076983	0.076313	0.076237	0.076248	0.076174	0.076137	0.076232	0.076207	0.076202

S7c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0894	1.0896	1.0907	1.0904	1.0863	1.0887	1.0888	1.0888	1.0878	1.0879	1.0864	1.0864	1.0864
R(1,3)	1.0888	1.0893	1.0905	1.0903	1.0858	1.0884	1.0886	1.0886	1.0876	1.0877	1.0862	1.0862	1.0862
R(1,4)	1.0932	1.0932	1.0941	1.0941	1.0898	1.0923	1.0925	1.0925	1.0913	1.0915	1.0899	1.0899	1.09
R(1,5)	1.9863	1.9581	1.9535	1.9582	1.9767	1.9622	1.9623	1.9624	1.9565	1.9565	1.956	1.9562	1.9563
R(5,10)	2.3173	2.1951	2.1949	2.1938	2.3196	2.2082	2.2079	2.2079	2.1846	2.1845	2.1832	2.183	2.183
R(6,7)	1.0923	1.0941	1.0946	1.0945	1.0888	1.0933	1.0934	1.0934	1.0927	1.0928	1.0913	1.0914	1.0914
R(6,8)	1.0905	1.0917	1.092	1.0919	1.0861	1.0902	1.0904	1.0903	1.0893	1.0894	1.088	1.088	1.0881
R(6,9)	1.0898	1.0911	1.0916	1.0914	1.0856	1.0896	1.0899	1.0899	1.0889	1.0891	1.0877	1.0877	1.0877
R(6,10)	1.8831	1.8257	1.8243	1.8237	1.8849	1.8226	1.8226	1.8227	1.8159	1.8158	1.8118	1.8122	1.8123
A(2,1,3)	111.5384	111.4285	110.6478	110.8743	110.6128	111.0109	111.0066	111.0276	110.9554	110.9599	110.978	110.9978	110.9984
A(2,1,4)	109.7864	109.5469	109.3282	109.4837	109.5917	109.6009	109.5848	109.5896	109.6027	109.5963	109.6478	109.6633	109.6692
A(2,1,5)	110.0585	110.4692	110.9961	111.3247	110.714	110.6239	110.6681	110.6708	110.6092	110.6431	110.549	110.5222	110.5267
A(3,1,4)	109.9918	109.7364	109.6678	109.8371	109.7465	109.8483	109.8279	109.8326	109.8734	109.8639	109.9043	109.9293	109.9296
A(3,1,5)	108.9941	109.5463	109.9074	109.6774	109.7044	109.6734	109.7043	109.7062	109.6582	109.681	109.6003	109.5924	109.5864
A(4,1,5)	106.3337	105.9656	106.1891	105.5036	106.38	105.9586	105.9226	105.8849	106.0232	105.9753	106.0426	106.0151	106.0097
A(1,5,10)	98.18	101.0272	100.7787	100.8126	99.1013	100.6367	100.7937	100.8137	101.1389	101.2561	101.089	101.1429	101.1494
A(7,6,8)	109.8416	109.0496	108.8783	109.0396	109.8299	109.0036	108.9927	108.9953	109.0403	109.0371	109.0038	109.0069	109.0075
A(7,6,9)	110.2098	109.3583	109.1681	109.2814	109.9536	109.2049	109.2059	109.2015	109.2711	109.2709	109.2124	109.2364	109.2382
A(7,6,10)	106.1905	106.2872	105.9959	106.2379	105.5728	105.8016	105.8161	105.8261	105.911	105.8654	105.8829	105.8355	105.8315
A(8,6,9)	110.6884	110.0729	110.1299	110.0178	110.8489	110.3158	110.2853	110.3116	110.3633	110.3606	110.353	110.3723	110.3667
A(8,6,10)	110.2501	111.438	111.5177	111.396	110.5636	111.4966	111.4776	111.4699	111.3821	111.3847	111.449	111.4257	111.4259
A(9,6,10)	109.5633	110.538	111.0245	110.7674	109.9424	110.8833	110.9296	110.9024	110.7462	110.7931	110.808	110.8304	110.8374
A(5,10,6)	98.4067	102.5542	103.3398	102.5203	101.508	103.3266	103.4033	103.3899	103.7256	103.8046	103.9606	103.9918	104.0006
D(2,1,5,10)	-63.0709	-65.0926	-66.2581	-60.1489	-65.3772	-65.1609	-65.5062	-65.4499	-65.3272	-65.5635	-65.5323	-65.4891	-65.5853
D(3,1,5,10)	59.5458	58.0231	56.4723	62.9327	56.9816	57.6182	57.318	57.404	57.3619	57.1694	57.1062	57.1512	57.0547
D(4,1,5,10)	178.0781	176.3364	175.0189	-178.8253	175.623	176.1257	175.7972	175.8685	175.9273	175.7086	175.689	175.7442	175.6416
D(1,5,10,6)	85.9915	87.2053	86.781	88.8111	88.2238	87.5723	87.5553	87.5717	87.4639	87.6172	87.5029	87.5151	87.5274
D(7,6,10,5)	174.8028	172.3858	175.4047	178.5536	176.5682	175.7861	176.0233	176.0707	175.845	175.8752	175.9163	175.9998	175.9855
D(8,6,10,5)	-66.2609	-68.9265	-66.2469	-62.8238	-64.7024	-65.8431	-65.6205	-65.5681	-65.7358	-65.7355	-65.6894	-65.643	-65.6589
D(9,6,10,5)	55.794	53.8157	56.9731	59.9811	58.0146	57.4999	57.7029	57.7641	57.4882	57.5205	57.6133	57.684	57.6662
Energy	-2877.04485566	-2877.31915726	-2877.33743288	-2877.33953937	-2879.44717763	-2879.52662452	-2879.52835282	-2879.52861387	-2879.53858058	-2879.54004269	-2879.54684904	-2879.54759156	-2879.54767171
ZPE Correction	0.077442	0.076782	0.07672	0.076651	0.076901	0.076235	0.076154	0.076163	0.07608	0.07604	0.076128	0.0761	0.076095

S7d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0963	1.096	1.0971	1.0969	1.0929	1.0948	1.095	1.0949	1.0939	1.0939	1.0924	1.0924	1.0924
R(1,3)	1.0952	1.0955	1.0967	1.0965	1.0922	1.0943	1.0945	1.0945	1.0935	1.0936	1.0921	1.0921	1.0921
R(1,4)	1.0997	1.0993	1.1003	1.1003	1.0962	1.0981	1.0983	1.0983	1.0971	1.0972	1.0957	1.0957	1.0957
R(1,5)	2.0276	1.9946	1.9903	1.996	2.0157	1.9987	1.999	1.9991	1.9926	1.993	1.9917	1.9921	1.9921
R(5,10)	2.3476	2.2185	2.2187	2.2175	2.3554	2.2362	2.2355	2.2354	2.2103	2.2097	2.2075	2.2071	2.2071
R(6,7)	1.0987	1.1001	1.1007	1.1007	1.095	1.099	1.0992	1.0992	1.0983	1.0985	1.0969	1.097	1.097
R(6,8)	1.0974	1.0979	1.0983	1.0982	1.0925	1.0961	1.0963	1.0963	1.0952	1.0953	1.0939	1.0939	1.0939
R(6,9)	1.0962	1.0972	1.0978	1.0975	1.0918	1.0954	1.0958	1.0958	1.0947	1.0949	1.0934	1.0935	1.0935
R(6,10)	1.9161	1.8506	1.8494	1.8489	1.9192	1.847	1.847	1.847	1.8404	1.8403	1.8351	1.8355	1.8355
A(2,1,3)	111.7302	111.5012	110.7916	111.0324	110.8919	111.1254	111.1358	111.1516	111.0696	111.0931	111.0897	111.1213	111.1225
A(2,1,4)	110.2554	109.9184	109.7058	109.8655	110.0041	109.951	109.9396	109.9436	109.9579	109.9598	109.9892	110.0141	110.0195
A(2,1,5)	109.23	109.8724	110.4106	110.6495	110.0863	110.0419	110.0892	110.0926	110.0396	110.0575	110.0087	109.9664	109.9721
A(3,1,4)	110.6313	110.1987	110.1273	110.3503	110.236	110.2775	110.2576	110.2613	110.2989	110.2983	110.3119	110.3463	110.3467
A(3,1,5)	108.4699	109.0964	109.4265	109.2081	109.1906	109.2305	109.2535	109.2555	109.2165	109.2261	109.1884	109.1661	109.1599
A(4,1,5)	106.352	106.1063	106.2798	105.5973	106.3263	106.0882	106.0368	106.0058	106.1369	106.0813	106.1293	106.0995	106.0927
A(1,5,10)	97.3925	100.6659	100.4244	100.4569	98.6225	100.3166	100.4686	100.4905	100.8139	100.9336	100.8296	100.8743	100.8816
A(7,6,8)	110.2815	109.4021	109.2437	109.4084	110.2541	109.3605	109.3477	109.3479	109.3971	109.3931	109.3405	109.3464	109.3479
A(7,6,9)	110.7831	109.7733	109.5781	109.7108	110.4599	109.6165	109.6116	109.6054	109.68	109.6769	109.6043	109.6262	109.6282
A(7,6,10)	106.183	106.3202	106.0024	106.2866	105.4674	105.7875	105.7986	105.8115	105.9241	105.8647	105.9028	105.8415	105.8394
A(8,6,9)	110.8782	110.1488	110.1971	110.0685	111.0878	110.4012	110.3684	110.39	110.415	110.4192	110.3879	110.4162	110.4115
A(8,6,10)	109.5534	110.9686	111.0363	110.8803	109.9543	111.0114	111.003	110.9996	110.8908	110.904	110.9804	110.9621	110.9619
A(9,6,10)	109.0388	110.1513	110.684	110.4101	109.466	110.5516	110.6009	110.5751	110.4295	110.4758	110.5176	110.538	110.5416
A(5,10,6)	97.6436	102.457	103.2213	102.362	101.0914	103.2915	103.3593	103.3518	103.7213	103.8055	103.9553	103.9852	103.9901
D(2,1,5,10)	-59.6369	-64.3617	-65.8425	-58.1968	-64.6968	-64.6507	-65.0448	-65.0363	-64.9782	-65.1362	-65.2251	-65.111	-65.2139
D(3,1,5,10)	62.3632	58.1562	56.3555	64.313	57.2625	57.5963	57.2605	57.2921	57.1888	57.0776	56.9289	57.0406	56.9388
D(4,1,5,10)	-178.6145	176.8599	175.2447	-177.028	176.182	176.4528	176.0768	176.0966	176.0903	175.9525	175.827	175.951	175.8426
D(1,5,10,6)	82.2845	85.2052	84.8711	86.7707	85.5202	85.5355	85.509	85.5026	85.5062	85.6868	85.5206	85.5441	85.5526
D(7,6,10,5)	176.2311	172.4951	176.0555	179.0032	177.4186	176.2611	176.457	176.4771	176.2559	176.3034	176.3031	176.452	176.44
D(8,6,10,5)	-64.6847	-68.6296	-65.4123	-62.1822	-63.7261	-65.2074	-65.0248	-64.9985	-65.1523	-65.1377	-65.1377	-65.0277	-65.0392
D(9,6,10,5)	56.8249	53.6178	57.3117	60.0809	58.5711	57.6673	57.8366	57.8701	57.5715	57.6327	57.6746	57.8224	57.8072
Energy	-2878.29597229	-2878.55796691	-2878.57759308	-2878.57972456	-2880.68601186	-2880.7588053	-2880.76047309	-2880.76066099	-2880.76947121	-2880.77099068	-2880.77696039	-2880.77775079	-2880.77781659
ZPE Correction	0.075001	0.074253	0.074174	0.074145	0.074236	0.073776	0.073692	0.073692	0.07365	0.073607	0.073711	0.073682	0.073678

S7e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0913	1.0912	1.0924	1.0921	1.0877	1.0901	1.0902	1.0902	1.0892	1.0893	1.0877	1.0877	1.0877
R(1,3)	1.0903	1.0908	1.092	1.0918	1.0871	1.0896	1.0898	1.0898	1.0888	1.0889	1.0874	1.0873	1.0874
R(1,4)	1.0948	1.0947	1.0957	1.0956	1.091	1.0935	1.0937	1.0937	1.0926	1.0927	1.0911	1.0911	1.0911
R(1,5)	1.9967	1.9692	1.9648	1.9697	1.9866	1.9728	1.9729	1.973	1.9671	1.9671	1.9667	1.967	1.967
R(5,10)	2.3259	2.2086	2.2085	2.2075	2.3287	2.221	2.2207	2.2206	2.1983	2.198	2.1971	2.1969	2.197
R(6,7)	1.0937	1.0954	1.096	1.0959	1.0898	1.0943	1.0944	1.0944	1.0938	1.0939	1.0923	1.0924	1.0924
R(6,8)	1.0924	1.0931	1.0935	1.0934	1.0874	1.0913	1.0915	1.0915	1.0905	1.0906	1.0891	1.0891	1.0891
R(6,9)	1.0913	1.0924	1.093	1.0928	1.0867	1.0907	1.091	1.0909	1.09	1.0902	1.0886	1.0887	1.0887
R(6,10)	1.8974	1.841	1.8397	1.8392	1.8991	1.8385	1.8384	1.8384	1.8301	1.83	1.8265	1.8269	1.8269
A(2,1,3)	111.5685	111.4658	110.725	110.9496	110.6965	111.0606	111.0646	111.0826	111.0146	111.027	111.0411	111.0624	111.0627
A(2,1,4)	109.9112	109.6902	109.463	109.6319	109.7239	109.7249	109.7086	109.7134	109.7286	109.7226	109.7649	109.7823	109.7866
A(2,1,5)	109.8046	110.2395	110.7581	111.0677	110.5017	110.3974	110.4393	110.4413	110.3852	110.4179	110.3426	110.3137	110.3185
A(3,1,4)	110.2269	109.928	109.8522	110.0334	109.9193	110.0176	109.9982	110.0024	110.0404	110.0324	110.0618	110.0878	110.0873
A(3,1,5)	108.8296	109.3663	109.7316	109.4646	109.5315	109.5045	109.5321	109.533	109.4977	109.5176	109.4588	109.4459	109.4415
A(4,1,5)	106.3576	106.0043	106.2091	105.557	106.3752	106.0125	105.9727	105.9406	106.0552	106.0015	106.0508	106.0258	106.0211
A(1,5,10)	97.7732	100.6717	100.4238	100.4514	98.853	100.2879	100.438	100.4578	100.7843	100.9104	100.7627	100.8173	100.8225
A(7,6,8)	110.0579	109.2818	109.1132	109.2776	110.0559	109.2543	109.2354	109.2393	109.2527	109.2442	109.2249	109.2241	109.2254
A(7,6,9)	110.5064	109.6369	109.4383	109.5513	110.2272	109.4948	109.4886	109.4852	109.5181	109.5141	109.4689	109.4864	109.4884
A(7,6,10)	106.1259	106.2106	105.93	106.1988	105.4796	105.7439	105.7565	105.7713	105.8742	105.8258	105.8415	105.7865	105.7839
A(8,6,9)	110.8399	110.2198	110.2784	110.1472	111.0125	110.4648	110.4393	110.4603	110.4827	110.4849	110.4764	110.4997	110.4955
A(8,6,10)	109.9192	111.1173	111.2119	111.0835	110.2635	111.1663	111.1518	111.1441	111.0896	111.0954	111.151	111.1342	111.1331
A(9,6,10)	109.2798	110.2855	110.7552	110.493	109.66	110.5934	110.6468	110.618	110.5063	110.5564	110.5573	110.5861	110.5909
A(5,10,6)	97.8993	102.2488	103.0313	102.1998	101.2926	103.0744	103.1411	103.1246	103.4232	103.5	103.6623	103.7024	103.7076
D(2,1,5,10)	-61.0613	-64.506	-65.6678	-59.4619	-65.0177	-64.7345	-65.0462	-65.0195	-64.8425	-65.0603	-65.0823	-65.028	-65.1202
D(3,1,5,10)	61.3244	58.3834	56.8801	63.3941	57.1905	57.8433	57.5828	57.6339	57.6652	57.4976	57.4048	57.4582	57.3666
D(4,1,5,10)	-179.9388	176.8514	175.5642	-178.2112	175.9425	176.4933	176.2018	176.2404	176.3625	176.1657	176.1046	176.1681	176.0709
D(1,5,10,6)	84.6075	86.6613	86.2333	88.2016	87.4534	86.9684	86.9282	86.9286	86.9368	87.0668	86.9745	86.9947	87.0029
D(7,6,10,5)	175.7444	172.9622	175.8469	178.9031	176.815	176.1903	176.435	176.484	176.3014	176.3714	176.31	176.4415	176.443
D(8,6,10,5)	-65.2755	-68.2919	-65.7263	-62.3815	-64.3974	-65.3488	-65.1269	-65.0687	-65.2032	-65.1689	-65.2147	-65.1255	-65.1247
D(9,6,10,5)	56.5704	54.2392	57.2746	60.1783	58.1357	57.7446	57.9615	58.0208	57.7982	57.8746	57.8575	57.985	57.9831
Energy	-2876.88773959	-2877.15912666	-2877.17811553	-2877.18024861	-2879.29443266	-2879.3722224	-2879.37389194	-2879.37410179	-2879.38395052	-2879.38537707	-2879.39183453	-2879.39259368	-2879.39266142
ZPE Correction	0.077185	0.076486	0.076392	0.076333	0.076578	0.075954	0.075872	0.075878	0.075837	0.075792	0.075869	0.075843	0.075841

S7f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0902	1.0903	1.0916	1.0912	1.0867	1.0893	1.0895	1.0895	1.0886	1.0888	1.0878	1.0878	1.0878
R(1,3)	1.0894	1.0899	1.0912	1.091	1.0861	1.0888	1.0891	1.0891	1.0882	1.0885	1.0875	1.0875	1.0875
R(1,4)	1.0939	1.0937	1.0948	1.0947	1.0903	1.0928	1.0931	1.0931	1.092	1.0922	1.0912	1.0912	1.0912
R(1,5)	1.9939	1.9611	1.9569	1.9616	1.9844	1.9675	1.968	1.968	1.962	1.9626	1.9611	1.9616	1.9616
R(5,10)	2.323	2.1889	2.1889	2.1877	2.3319	2.2074	2.2069	2.2068	2.1817	2.1811	2.1788	2.1786	2.1786
R(6,7)	1.0933	1.0948	1.0954	1.0954	1.0893	1.0939	1.0941	1.0941	1.0936	1.0938	1.0926	1.0927	1.0927
R(6,8)	1.0915	1.0926	1.0931	1.0929	1.0867	1.0909	1.0913	1.0913	1.0904	1.0907	1.0897	1.0897	1.0897
R(6,9)	1.0906	1.0918	1.0925	1.0922	1.086	1.0901	1.0906	1.0906	1.0897	1.0901	1.0891	1.0891	1.0891
R(6,10)	1.8827	1.8215	1.8206	1.8199	1.8853	1.8191	1.819	1.819	1.8143	1.8142	1.8088	1.8089	1.8089
A(2,1,3)	111.6054	111.3262	110.5714	110.83	110.751	110.9996	111.0212	111.0298	110.9253	110.9624	110.9357	110.9621	110.9651
A(2,1,4)	109.7883	109.4442	109.2277	109.3598	109.6143	109.5651	109.5488	109.5471	109.5816	109.58	109.5853	109.6035	109.607
A(2,1,5)	110.0663	110.6094	111.1735	111.5426	110.8158	110.7468	110.7793	110.7869	110.7233	110.7387	110.7398	110.7069	110.7126
A(3,1,4)	110.0521	109.6767	109.5887	109.7422	109.7662	109.8384	109.8166	109.8213	109.8725	109.8713	109.859	109.8887	109.8861
A(3,1,5)	109.1028	109.7878	110.1513	109.9244	109.8337	109.8621	109.8885	109.8999	109.8575	109.8672	109.8642	109.8369	109.8339
A(4,1,5)	106.0732	105.8468	106.0153	105.2892	105.9461	105.6926	105.6464	105.614	105.7517	105.6875	105.7261	105.7105	105.7034
A(1,5,10)	98.819	101.6558	101.5197	101.5852	100.1924	101.4904	101.614	101.6426	101.9557	102.0972	101.997	102.0418	102.0487
A(7,6,8)	109.7407	108.8708	108.705	108.8452	109.7654	108.897	108.8644	108.8628	108.9031	108.8994	108.854	108.8398	108.8421
A(7,6,9)	110.1049	109.1996	109.0259	109.1274	109.9034	109.132	109.1153	109.1057	109.1732	109.1754	109.1087	109.1093	109.1119
A(7,6,10)	105.8478	106.0281	105.762	105.9776	105.1775	105.459	105.4772	105.4976	105.6707	105.6064	105.6073	105.5426	105.5457
A(8,6,9)	110.6603	109.9707	110.0351	109.9419	110.9194	110.3207	110.2842	110.2963	110.305	110.3206	110.2643	110.2958	110.2916
A(8,6,10)	110.4618	111.6871	111.7796	111.6996	110.7356	111.6914	111.7052	111.7021	111.5815	111.5975	111.6983	111.7055	111.7016
A(9,6,10)	109.9176	110.9653	111.3817	111.1236	110.1873	111.179	111.2327	111.2146	111.0602	111.0904	111.1535	111.1878	111.1884
A(5,10,6)	99.573	103.6976	104.4382	103.6691	102.7624	104.5583	104.5964	104.5809	104.7915	104.8653	105.0951	105.1396	105.1353
D(2,1,5,10)	-63.1328	-65.2085	-66.3415	-60.7113	-65.9337	-65.3873	-65.5468	-65.5418	-65.4437	-65.4487	-65.7231	-65.6247	-65.71
D(3,1,5,10)	59.6437	58.0369	56.5823	62.6377	56.7553	57.5889	57.4968	57.5257	57.4195	57.4783	57.1689	57.2599	57.1801
D(4,1,5,10)	178.1599	176.338	175.0641	-179.2263	175.2419	176.0326	175.9024	175.9244	175.9344	175.9606	175.6569	175.7601	175.6717
D(1,5,10,6)	85.229	86.5117	86.2485	88.241	87.5187	87.052	86.9698	86.9486	86.974	87.085	86.8983	86.9634	86.9736
D(7,6,10,5)	175.1618	173.0622	175.7536	178.2045	176.5317	175.8916	176.1595	176.1325	175.9468	176.0976	175.8637	176.1751	176.1807
D(8,6,10,5)	-66.1087	-68.4874	-66.1071	-63.3999	-64.9554	-65.9676	-65.7207	-65.739	-65.8364	-65.7201	-65.9545	-65.6953	-65.6869
D(9,6,10,5)	56.2858	54.6054	57.441	59.7795	58.1354	57.7384	57.9875	57.9693	57.6821	57.8523	57.6643	57.9951	57.9955
Energy	-2878.47924362	-2878.74683194	-2878.76748569	-2878.76959256	-2880.86758837	-2880.94539413	-2880.94725928	-2880.94740954	-2880.95609273	-2880.95782759	-2880.96352725	-2880.96440034	-2880.96447234
ZPE Correction	0.076594	0.075966	0.075885	0.075841	0.076186	0.07551	0.075402	0.0754	0.075268	0.075199	0.075244	0.075226	0.075228

S7g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0892	1.0894	1.0906	1.0903	1.086	1.0886	1.0888	1.0888	1.0879	1.0881	1.0869	1.0869	1.0869
R(1,3)	1.0887	1.0891	1.0904	1.0902	1.0855	1.0882	1.0885	1.0885	1.0876	1.0878	1.0867	1.0867	1.0867
R(1,4)	1.0932	1.0931	1.0941	1.0941	1.0897	1.0923	1.0926	1.0926	1.0915	1.0918	1.0906	1.0906	1.0906
R(1,5)	1.9916	1.9612	1.9569	1.9614	1.9819	1.9663	1.9667	1.9668	1.9609	1.9613	1.9601	1.9606	1.9607
R(5,10)	2.3202	2.1939	2.1935	2.1922	2.3244	2.2088	2.2083	2.2082	2.185	2.1845	2.183	2.1828	2.1828
R(6,7)	1.0924	1.094	1.0946	1.0946	1.0886	1.0931	1.0934	1.0934	1.0929	1.0932	1.0918	1.0919	1.0919
R(6,8)	1.0903	1.0916	1.092	1.0918	1.0859	1.09	1.0904	1.0904	1.0894	1.0897	1.0886	1.0886	1.0886
R(6,9)	1.0897	1.0909	1.0915	1.0913	1.0853	1.0894	1.0899	1.0899	1.0889	1.0892	1.0881	1.0881	1.0881
R(6,10)	1.8867	1.8278	1.8266	1.8261	1.8888	1.8254	1.8253	1.8254	1.8192	1.8192	1.8148	1.815	1.815
A(2,1,3)	111.6053	111.3849	110.6326	110.8749	110.7138	111.0173	111.028	111.0401	110.9571	110.9859	110.963	110.9934	110.994
A(2,1,4)	109.8232	109.4965	109.2862	109.4399	109.6146	109.5852	109.5742	109.5725	109.5981	109.598	109.6048	109.629	109.6317
A(2,1,5)	110.1018	110.577	111.1248	111.4982	110.7969	110.74	110.7803	110.7876	110.7154	110.7421	110.7245	110.6864	110.6916
A(3,1,4)	109.9912	109.6889	109.6092	109.7554	109.7598	109.8306	109.8093	109.8142	109.8627	109.8576	109.852	109.8842	109.8828
A(3,1,5)	109.0916	109.7405	110.1081	109.8426	109.84	109.8499	109.8753	109.8857	109.834	109.8464	109.8376	109.8054	109.8048
A(4,1,5)	106.0747	105.7985	105.964	105.2757	106.0061	105.6802	105.6329	105.5977	105.7425	105.6752	105.7268	105.7085	105.7017
A(1,5,10)	98.8354	101.5821	101.4618	101.5052	100.0616	101.3847	101.5177	101.5424	101.8237	101.9689	101.8583	101.9018	101.9098
A(7,6,8)	109.8564	109.0057	108.845	108.9811	109.8666	109.0236	108.9985	108.9967	109.0232	109.0262	108.9793	108.9777	108.9786
A(7,6,9)	110.1709	109.29	109.1077	109.207	109.9756	109.2138	109.1978	109.1887	109.2449	109.2488	109.1833	109.1925	109.1943
A(7,6,10)	105.8395	106.0084	105.7417	105.9516	105.2001	105.4607	105.4734	105.4905	105.627	105.557	105.5923	105.5202	105.5191
A(8,6,9)	110.7628	110.0837	110.1366	110.0505	110.9582	110.3887	110.3474	110.3657	110.3998	110.4046	110.3617	110.3915	110.3874
A(8,6,10)	110.3701	111.5675	111.6672	111.5845	110.643	111.5858	111.6007	111.596	111.4953	111.5135	111.5915	111.5928	111.5916
A(9,6,10)	109.7281	110.7719	111.1986	110.9462	110.0456	111.0139	111.0691	111.0491	110.9063	110.9427	110.9832	111.012	111.016
A(5,10,6)	99.4489	103.4123	104.18	103.4121	102.5576	104.3066	104.3588	104.3403	104.5432	104.6335	104.8253	104.8771	104.8782
D(2,1,5,10)	-64.0183	-65.1494	-66.2653	-61.0621	-65.6895	-65.4097	-65.6755	-65.6245	-65.4983	-65.659	-65.7933	-65.7821	-65.8463
D(3,1,5,10)	58.7738	58.1159	56.6728	62.2555	56.944	57.5759	57.3683	57.4468	57.3836	57.2858	57.1047	57.1067	57.0463
D(4,1,5,10)	177.2133	176.3799	175.1269	-179.6415	175.4603	175.9971	175.7509	175.8207	175.8696	175.7343	175.5711	175.5842	175.518
D(1,5,10,6)	86.6568	87.3631	87.0999	89.0013	88.4419	87.7754	87.7367	87.7357	87.6917	87.8088	87.6587	87.691	87.7033
D(7,6,10,5)	174.4199	172.9438	175.3908	178.0634	176.193	175.6382	175.8197	175.8256	175.804	175.8237	175.674	175.8551	175.8364
D(8,6,10,5)	-66.7661	-68.5202	-66.3739	-63.4553	-65.2086	-66.1241	-65.9572	-65.9456	-65.907	-65.916	-66.0595	-65.9228	-65.9417
D(9,6,10,5)	55.5696	54.4937	57.0895	59.6533	57.7707	57.4723	57.6368	57.654	57.5602	57.597	57.4836	57.6808	57.6587
Energy	-2877.56896948	-2877.83906603	-2877.8592718	-2877.86135335	-2879.96812502	-2880.0470602	-2880.04901735	-2880.04920627	-2880.0582577	-2880.06008052	-2880.06583774	-2880.06673064	-2880.06680044
ZPE Correction	0.077245	0.076614	0.07651	0.076423	0.076758	0.07609	0.075976	0.075974	0.075876	0.075806	0.075855	0.075825	0.075822

S7h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0977	1.0973	1.0986	1.0982	1.0941	1.096	1.0962	1.0962	1.0952	1.0953	1.0939	1.0938	1.0939
R(1,3)	1.0967	1.0968	1.0983	1.098	1.0935	1.0956	1.0958	1.0958	1.0948	1.095	1.0936	1.0936	1.0936
R(1,4)	1.1014	1.1009	1.1021	1.102	1.0977	1.0997	1.0999	1.0999	1.0987	1.0989	1.0974	1.0975	1.0975
R(1,5)	2.003	1.9744	1.9702	1.9751	1.9944	1.9792	1.9794	1.9795	1.9733	1.9735	1.9726	1.973	1.9731
R(5,10)	2.3343	2.2078	2.2079	2.2068	2.3394	2.2229	2.2224	2.2223	2.1985	2.198	2.1965	2.1962	2.1962
R(6,7)	1.1005	1.1019	1.1027	1.1026	1.0968	1.1008	1.101	1.101	1.1003	1.1005	1.099	1.0991	1.0991
R(6,8)	1.099	1.0994	1.1	1.0999	1.0939	1.0976	1.0978	1.0978	1.0968	1.097	1.0956	1.0957	1.0957
R(6,9)	1.0978	1.0988	1.0995	1.0993	1.0933	1.097	1.0973	1.0973	1.0963	1.0965	1.0952	1.0952	1.0952
R(6,10)	1.8979	1.8386	1.8374	1.8369	1.9009	1.8356	1.8355	1.8355	1.8285	1.8284	1.8241	1.8245	1.8245
A(2,1,3)	111.6449	111.5633	110.7869	111.0385	110.8098	111.1626	111.1693	111.1878	111.1295	111.1501	111.1533	111.1835	111.1834
A(2,1,4)	109.869	109.6574	109.4067	109.5571	109.6873	109.6968	109.678	109.6823	109.7312	109.7277	109.7684	109.7915	109.7959
A(2,1,5)	109.8443	110.3103	110.8953	111.2173	110.6176	110.4867	110.542	110.5457	110.439	110.475	110.4031	110.3633	110.3681
A(3,1,4)	110.2045	109.8786	109.7749	109.9638	109.8551	109.9748	109.9483	109.9527	110.0344	110.0244	110.0515	110.0851	110.0845
A(3,1,5)	108.8941	109.3974	109.7767	109.5384	109.5804	109.5263	109.5548	109.5575	109.4752	109.4944	109.4397	109.4174	109.4152
A(4,1,5)	106.2333	105.8755	106.089	105.3741	106.185	105.858	105.8101	105.774	105.8998	105.8337	105.8914	105.8638	105.8572
A(1,5,10)	97.9148	101.0507	100.8361	100.8836	99.2038	100.6867	100.849	100.8763	101.1392	101.2857	101.1448	101.1924	101.1999
A(7,6,8)	109.937	109.1145	108.9172	109.0734	109.9143	109.0656	109.0402	109.0427	109.1175	109.1098	109.079	109.0775	109.0791
A(7,6,9)	110.4031	109.4556	109.2321	109.3541	110.0598	109.2876	109.2775	109.272	109.3734	109.3685	109.315	109.3311	109.3333
A(7,6,10)	106.1078	106.1854	105.8755	106.1457	105.3854	105.661	105.6735	105.6905	105.7839	105.7224	105.7506	105.6824	105.6806
A(8,6,9)	110.7941	110.1705	110.2118	110.0826	111.0035	110.4238	110.3896	110.4131	110.4704	110.4783	110.4614	110.4917	110.4866
A(8,6,10)	110.0734	111.3641	111.4764	111.3479	110.476	111.4306	111.4292	111.4229	111.291	111.3038	111.3642	111.3511	111.3503
A(9,6,10)	109.4187	110.4523	110.9976	110.7346	109.8563	110.8323	110.8914	110.8601	110.6746	110.7241	110.7356	110.7679	110.772
A(5,10,6)	97.8395	102.5908	103.4232	102.5643	101.4718	103.4388	103.5163	103.5013	103.7828	103.8737	104.0461	104.0871	104.0902
D(2,1,5,10)	-60.4027	-64.9765	-66.3447	-60.0448	-65.4593	-65.2186	-65.6476	-65.6372	-65.3879	-65.6306	-65.6791	-65.5907	-65.6618
D(3,1,5,10)	62.1443	58.1026	56.4041	63.0754	56.9999	57.5608	57.1962	57.2341	57.2842	57.1039	56.9754	57.0607	56.9911
D(4,1,5,10)	-179.1801	176.4569	174.9521	-178.6753	175.5942	176.0851	175.6772	175.7016	175.8758	175.6566	175.5641	175.6621	175.5871
D(1,5,10,6)	84.2908	86.5395	86.2848	88.1506	87.3408	86.9256	86.892	86.8871	86.9164	87.0714	86.9359	86.9633	86.9724
D(7,6,10,5)	175.9136	172.2568	175.4949	178.4234	176.5089	175.6874	175.8763	175.8964	175.7562	175.7947	175.7537	175.9311	175.9259
D(8,6,10,5)	-65.1785	-69.0794	-66.2045	-62.9951	-64.8153	-65.9868	-65.8216	-65.7918	-65.8568	-65.8573	-65.8863	-65.7582	-65.763
D(9,6,10,5)	56.7991	53.6758	57.0723	59.8358	57.9795	57.4115	57.5743	57.6073	57.3893	57.4433	57.4437	57.6246	57.6157
Energy	-2876.45055818	-2876.72244808	-2876.74267425	-2876.74481238	-2878.85033713	-2878.92638778	-2878.92818249	-2878.92838309	-2878.93777178	-2878.93937811	-2878.94565034	-2878.94649279	-2878.94656167
ZPE Correction	0.075368	0.074613	0.074502	0.074422	0.074732	0.074078	0.073978	0.073979	0.073923	0.073867	0.073964	0.073932	0.073928

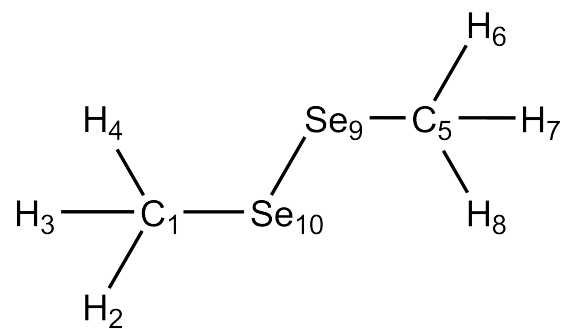
S7i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0917	1.0917	1.0928	1.0925	1.0881	1.0903	1.0904	1.0904	1.0893	1.0894	1.0877	1.0877	1.0877
R(1,3)	1.0909	1.0913	1.0925	1.0922	1.0875	1.0899	1.0901	1.0901	1.089	1.0891	1.0875	1.0874	1.0874
R(1,4)	1.0954	1.0952	1.0961	1.0961	1.0915	1.0938	1.094	1.094	1.0928	1.0929	1.0912	1.0912	1.0912
R(1,5)	1.9962	1.9677	1.9632	1.9681	1.9852	1.9708	1.9709	1.971	1.9653	1.9652	1.9647	1.965	1.965
R(5,10)	2.3235	2.2045	2.2044	2.2034	2.3281	2.2171	2.2168	2.2167	2.1939	2.1937	2.1923	2.1921	2.1921
R(6,7)	1.0943	1.0959	1.0965	1.0964	1.0904	1.0946	1.0948	1.0948	1.094	1.0942	1.0925	1.0925	1.0925
R(6,8)	1.0928	1.0936	1.094	1.0939	1.0878	1.0916	1.0918	1.0918	1.0908	1.0909	1.0893	1.0893	1.0893
R(6,9)	1.0919	1.093	1.0935	1.0933	1.0872	1.091	1.0913	1.0913	1.0902	1.0904	1.0888	1.0888	1.0888
R(6,10)	1.8952	1.8386	1.8372	1.8367	1.8964	1.8354	1.8353	1.8353	1.8268	1.8267	1.8232	1.8237	1.8237
A(2,1,3)	111.6139	111.4939	110.739	110.9634	110.7372	111.0983	111.098	111.1175	111.0517	111.0595	111.0725	111.0958	111.097
A(2,1,4)	109.919	109.6896	109.4583	109.6333	109.7228	109.7364	109.7186	109.7247	109.7405	109.7338	109.7793	109.7977	109.8031
A(2,1,5)	109.8896	110.2839	110.8096	111.136	110.5362	110.4292	110.4747	110.4767	110.4081	110.4411	110.3547	110.3238	110.3276
A(3,1,4)	110.1863	109.9036	109.8273	110.0037	109.9086	110.0052	109.9857	109.9899	110.0318	110.0235	110.0586	110.0853	110.0858
A(3,1,5)	108.8494	109.3959	109.7809	109.493	109.5671	109.527	109.5564	109.5549	109.512	109.5321	109.4709	109.4584	109.4531
A(4,1,5)	106.2329	105.9219	106.1194	105.4695	106.2706	105.9153	105.8762	105.8434	105.9722	105.9241	105.9795	105.9521	105.9463
A(1,5,10)	98.0619	100.8494	100.6207	100.6296	99.0279	100.5008	100.6533	100.6718	100.9816	101.0908	100.941	100.991	100.9967
A(7,6,8)	110.0215	109.2438	109.0781	109.2322	110.0135	109.2175	109.204	109.2064	109.2259	109.2209	109.1955	109.2003	109.2018
A(7,6,9)	110.434	109.579	109.379	109.4888	110.1599	109.4283	109.4283	109.4243	109.4622	109.4611	109.4081	109.4326	109.4346
A(7,6,10)	106.0692	106.1902	105.9115	106.1734	105.4425	105.7171	105.7304	105.7421	105.8384	105.7926	105.8157	105.7652	105.7616
A(8,6,9)	110.8282	110.2114	110.2598	110.1365	111.0013	110.4618	110.4341	110.4578	110.4745	110.4759	110.4695	110.4927	110.4881
A(8,6,10)	110.03	111.1968	111.2925	111.1654	110.3466	111.2462	111.2273	111.2204	111.1718	111.1724	111.228	111.203	111.2028
A(9,6,10)	109.3466	110.3277	110.8024	110.5514	109.7344	110.642	110.6902	110.6629	110.5469	110.5945	110.5992	110.6199	110.6251
A(5,10,6)	98.1342	102.3516	103.1377	102.319	101.3792	103.1873	103.2638	103.2523	103.5927	103.6695	103.8107	103.8406	103.8474
D(2,1,5,10)	-61.6836	-64.561	-65.6686	-59.859	-64.9266	-64.7873	-65.1502	-65.1364	-64.922	-65.1615	-65.0886	-65.0272	-65.1147
D(3,1,5,10)	60.825	58.4126	56.9649	63.0799	57.3789	57.8739	57.5604	57.599	57.6568	57.4622	57.4537	57.5158	57.4286
D(4,1,5,10)	179.4558	176.8213	175.5945	-178.5943	176.0779	176.4665	176.1234	176.1478	176.3048	176.084	176.1162	176.1879	176.0953
D(1,5,10,6)	85.4926	86.9842	86.5933	88.558	87.7792	87.3035	87.2819	87.2874	87.2319	87.3676	87.2673	87.2745	87.283
D(7,6,10,5)	175.1652	172.8255	175.6384	178.7229	176.6903	175.9301	176.1535	176.2103	175.9948	176.0507	176.06	176.1539	176.142
D(8,6,10,5)	-65.8718	-68.4433	-65.9448	-62.587	-64.5506	-65.6266	-65.4215	-65.3586	-65.5193	-65.4964	-65.4741	-65.4177	-65.4301
D(9,6,10,5)	56.0736	54.161	57.1227	60.0563	58.073	57.5536	57.7441	57.8132	57.5575	57.6163	57.6728	57.756	57.7412
Energy	-2877.23750787	-2877.50824838	-2877.52697477	-2877.5291012	-2879.6375375	-2879.71376594	-2879.71544529	-2879.71567501	-2879.72560388	-2879.72705063	-2879.73384064	-2879.73458163	-2879.73465194
ZPE Correction	0.076799	0.076148	0.076065	0.076013	0.076229	0.075633	0.075548	0.075554	0.075527	0.075486	0.075588	0.075562	0.075558

S7j – QCISD

	QCISD/cc-pvdz
R(1,2)	1.1019
R(1,3)	1.1011
R(1,4)	1.1044
R(1,5)	1.9638
R(5,10)	2.2205
R(6,7)	1.1048
R(6,8)	1.1027
R(6,9)	1.1018
R(6,10)	1.8333
A(2,1,3)	110.4547
A(2,1,4)	109.3995
A(2,1,5)	110.5754
A(3,1,4)	109.7989
A(3,1,5)	109.8646
A(4,1,5)	106.6722
A(1,5,10)	98.9005
A(7,6,8)	109.0353
A(7,6,9)	109.4170
A(7,6,10)	106.3153
A(8,6,9)	110.0061
A(8,6,10)	111.1932
A(9,6,10)	110.7818
A(5,10,6)	101.5272
D(2,1,5,10)	-63.3490
D(3,1,5,10)	58.8269
D(4,1,5,10)	177.7842
D(1,5,10,6)	86.0811
D(7,6,10,5)	178.6425
D(8,6,10,5)	-62.8038
D(9,6,10,5)	59.8539
Energy	-2877.1908209
ZPE Correction	0.076759

S8 – MeSSMe



S8a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0901	1.0915	1.092	1.092	1.0851	1.0896	1.0898	1.0897	1.0885	1.0887	1.087	1.087	1.087
R(1,3)	1.0895	1.0908	1.0915	1.0915	1.0844	1.089	1.0892	1.0892	1.088	1.0882	1.0866	1.0866	1.0866
R(1,4)	1.093	1.0939	1.0944	1.0943	1.088	1.0922	1.0924	1.0924	1.0916	1.0917	1.09	1.0901	1.0901
R(1,10)	1.8962	1.8361	1.8361	1.836	1.8974	1.833	1.8334	1.8334	1.8275	1.8276	1.8231	1.8235	1.8235
R(5,6)	1.093	1.0939	1.0944	1.0943	1.088	1.0922	1.0924	1.0924	1.0916	1.0917	1.09	1.0901	1.0901
R(5,7)	1.0901	1.0915	1.092	1.092	1.0851	1.0896	1.0898	1.0898	1.0885	1.0887	1.087	1.087	1.087
R(5,8)	1.0895	1.0908	1.0915	1.0915	1.0844	1.089	1.0892	1.0892	1.088	1.0882	1.0866	1.0866	1.0866
R(5,9)	1.8962	1.8361	1.8361	1.836	1.8974	1.833	1.8334	1.8334	1.8275	1.8276	1.8231	1.8235	1.8235
R(9,10)	2.2459	2.0822	2.0832	2.0833	2.2525	2.0936	2.0927	2.0925	2.0623	2.0619	2.0533	2.0533	2.0534
A(2,1,3)	110.9636	110.2945	110.2746	110.2648	111.0099	110.3253	110.3219	110.3556	110.4675	110.4589	110.45	110.4495	110.4443
A(2,1,4)	110.0099	109.0869	109.0491	109.0494	110.0298	109.1301	109.1128	109.1188	109.1496	109.1476	109.1258	109.1325	109.136
A(2,1,10)	110.4511	111.402	111.4815	111.4758	110.4607	111.4006	111.4011	111.3957	111.2861	111.3049	111.3275	111.3139	111.3186
A(3,1,4)	110.1846	109.401	109.3505	109.3526	110.173	109.4229	109.4107	109.417	109.4708	109.4679	109.454	109.4708	109.4708
A(3,1,10)	109.6909	110.6647	110.6627	110.6452	109.5793	110.5564	110.6075	110.5613	110.4301	110.4861	110.4897	110.5018	110.5029
A(4,1,10)	105.3988	105.8724	105.9018	105.9343	105.4446	105.8881	105.8676	105.8725	105.9177	105.8535	105.872	105.8505	105.8465
A(6,5,7)	110.0088	109.0862	109.0487	109.0492	110.027	109.1305	109.1132	109.1192	109.1501	109.1481	109.1264	109.133	109.1365
A(6,5,8)	110.1878	109.4017	109.351	109.3531	110.1791	109.4238	109.4114	109.4177	109.4715	109.4687	109.4549	109.4717	109.4717
A(6,5,9)	105.4001	105.8697	105.899	105.9312	105.4435	105.8842	105.8636	105.8685	105.9148	105.8508	105.8694	105.8475	105.8436
A(7,5,8)	110.9648	110.2945	110.2747	110.265	111.0106	110.3257	110.3225	110.3561	110.4679	110.4593	110.4506	110.45	110.4449
A(7,5,9)	110.4449	111.4042	111.4841	111.4789	110.4538	111.4028	111.4039	111.3986	111.2887	111.307	111.3294	111.3159	111.3206
A(8,5,9)	109.6924	110.665	110.6626	110.6447	109.5834	110.5561	110.6067	110.5605	110.4287	110.4849	110.4883	110.5004	110.5016
A(5,9,10)	101.2468	103.4323	103.4167	103.4013	100.5914	102.7524	102.9441	102.9472	103.6031	103.7634	103.959	103.9595	103.9668
A(1,10,9)	101.2495	103.4321	103.4174	103.4023	100.5922	102.7542	102.9463	102.9492	103.6045	103.7647	103.9604	103.9611	103.9684
D(2,1,10,9)	-64.8979	-65.0781	-65.3077	-65.4093	-64.3892	-64.9304	-64.8742	-65.0431	-65.7211	-65.502	-65.6898	-65.4952	-65.5702
D(3,1,10,9)	57.7185	58.0132	57.8128	57.682	58.2168	58.1223	58.2108	58.0485	57.3441	57.605	57.4242	57.6171	57.5395
D(4,1,10,9)	176.3182	176.4594	176.2149	176.0963	176.7718	176.5465	176.6355	176.4593	175.7761	176.0259	175.8411	176.0478	175.9685
D(6,5,9,10)	176.3218	176.4025	176.1638	176.0549	176.8016	176.5624	176.6486	176.4704	175.833	176.0711	175.9096	176.1091	176.0294
D(7,5,9,10)	-64.898	-65.1362	-65.3596	-65.4512	-64.367	-64.9151	-64.8615	-65.0324	-65.6639	-65.4567	-65.6211	-65.4339	-65.5093
D(8,5,9,10)	57.7168	57.957	57.7628	57.6421	58.2381	58.1395	58.2257	58.0614	57.4026	57.6515	57.4939	57.6797	57.6017
D(5,9,10,1)	88.9307	87.3762	87.5944	87.4548	90.0556	87.6279	87.8609	87.8065	87.0732	87.4543	87.2436	87.423	87.4046
Energy	-876.133422182	-876.215993024	-876.220392104	-876.220530556	-876.208418304	-876.284510006	-876.286906219	-876.287215882	-876.303878075	-876.305776723	-876.310633216	-876.311403798	-876.311472104
ZPE Correction	0.077966	0.077668	0.077409	0.0774	0.077385	0.077182	0.07705	0.077054	0.077024	0.076947	0.077071	0.07704	0.077031

S8b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0898	1.0913	1.0916	1.0916	1.0854	1.0898	1.0899	1.0899	1.0888	1.0889	1.0874	1.0874	1.0874
R(1,3)	1.0892	1.0907	1.0912	1.0912	1.0847	1.0892	1.0894	1.0894	1.0883	1.0885	1.087	1.087	1.087
R(1,4)	1.0926	1.0935	1.0939	1.0938	1.0882	1.0922	1.0924	1.0924	1.0917	1.0919	1.0903	1.0904	1.0904
R(1,10)	1.8792	1.8208	1.8204	1.8204	1.8784	1.8172	1.8177	1.8176	1.812	1.8122	1.808	1.8084	1.8084
R(5,6)	1.0926	1.0935	1.0939	1.0938	1.0882	1.0922	1.0924	1.0924	1.0917	1.0919	1.0903	1.0904	1.0904
R(5,7)	1.0898	1.0913	1.0917	1.0916	1.0854	1.0898	1.0899	1.0899	1.0888	1.0889	1.0874	1.0874	1.0874
R(5,8)	1.0892	1.0907	1.0912	1.0912	1.0847	1.0892	1.0894	1.0894	1.0883	1.0885	1.087	1.087	1.087
R(5,9)	1.8792	1.8207	1.8204	1.8204	1.8784	1.8172	1.8177	1.8176	1.812	1.8122	1.808	1.8084	1.8084
R(9,10)	2.2247	2.0615	2.0624	2.0625	2.2283	2.0708	2.0706	2.0704	2.0411	2.0413	2.033	2.0333	2.0334
A(2,1,3)	110.841	110.2213	110.1866	110.1882	110.8054	110.2195	110.2249	110.2667	110.4345	110.4258	110.4227	110.4203	110.4141
A(2,1,4)	109.8126	108.9026	108.8586	108.8807	109.7993	108.9571	108.9457	108.9533	109.0109	109.013	108.9949	109.0027	109.0071
A(2,1,10)	110.6457	111.559	111.6262	111.6135	110.6893	111.5442	111.5342	111.5281	111.4077	111.4181	111.4279	111.4092	111.4142
A(3,1,4)	109.9934	109.2314	109.1776	109.1987	109.9551	109.2671	109.2605	109.2673	109.3412	109.3438	109.3412	109.3614	109.3617
A(3,1,10)	109.8277	110.7546	110.7678	110.7316	109.7686	110.6636	110.7016	110.649	110.4903	110.5414	110.5404	110.5487	110.5493
A(4,1,10)	105.5922	106.0495	106.1008	106.107	105.7006	106.0715	106.0546	106.0565	106.0349	105.9749	105.9902	105.9752	105.9714
A(6,5,7)	109.8144	108.8976	108.8547	108.88	109.8	108.9574	108.9452	108.9531	109.0105	109.0126	108.9944	109.0023	109.0067
A(6,5,8)	109.9944	109.2375	109.1829	109.1996	109.9555	109.2669	109.2613	109.268	109.3413	109.344	109.3414	109.3617	109.362
A(6,5,9)	105.5964	106.0397	106.0922	106.1048	105.701	106.0712	106.0523	106.054	106.0344	105.9744	105.9897	105.9747	105.9708
A(7,5,8)	110.8422	110.2224	110.1878	110.1883	110.8057	110.2196	110.2251	110.2669	110.4343	110.4257	110.4226	110.4202	110.4139
A(7,5,9)	110.638	111.549	111.6168	111.6149	110.6878	111.5463	111.5354	111.5298	111.4089	111.4194	111.4288	111.4105	111.4154
A(8,5,9)	109.8274	110.7717	110.7829	110.7321	109.7683	110.6618	110.702	110.6489	110.4899	110.5409	110.5402	110.5483	110.5489
A(5,9,10)	101.0724	103.3168	103.2867	103.2925	100.2648	102.5784	102.7745	102.7801	103.4786	103.637	103.8322	103.823	103.8317
A(1,10,9)	101.0776	103.3145	103.2853	103.2919	100.266	102.5789	102.7747	102.7806	103.478	103.6364	103.8317	103.8226	103.8312
D(2,1,10,9)	-65.2398	-65.3923	-65.5169	-65.6574	-64.3399	-65.0037	-64.9546	-65.1714	-65.9575	-65.7445	-65.8582	-65.6744	-65.7503
D(3,1,10,9)	57.4444	57.7804	57.6685	57.4948	58.2885	58.0909	58.1671	57.962	57.1932	57.4389	57.3273	57.5009	57.4209
D(4,1,10,9)	175.997	176.1754	176.0363	175.8722	176.8265	176.4931	176.5716	176.3479	175.5705	175.8115	175.7051	175.8986	175.8169
D(6,5,9,10)	175.983	176.1654	176.0498	175.8801	176.8213	176.5118	176.5493	176.3551	175.563	175.8105	175.6971	175.9	175.8154
D(7,5,9,10)	-65.2533	-65.4196	-65.5185	-65.651	-64.3447	-64.9838	-64.9782	-65.1649	-65.9651	-65.7456	-65.8664	-65.6731	-65.752
D(8,5,9,10)	57.4271	57.7598	57.6726	57.5027	58.2829	58.111	58.1449	57.9699	57.186	57.4383	57.3195	57.5026	57.4196
D(5,9,10,1)	88.7869	87.2073	87.3662	87.1669	89.8812	87.2898	87.5884	87.5307	86.7923	87.2348	86.9826	87.1629	87.1467
Energy	-877.066750228	-877.151124772	-877.154054346	-877.154196747	-877.137048798	-877.21589824	-877.218576345	-877.218951813	-877.236471221	-877.238567288	-877.243047953	-877.243884694	-877.243966815
ZPE Correction	0.078424	0.077984	0.077775	0.077767	0.077847	0.077486	0.077364	0.077373	0.077273	0.077214	0.077305	0.077279	0.077269

S8c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0903	1.0918	1.0922	1.0922	1.0861	1.0904	1.0906	1.0905	1.0894	1.0896	1.0882	1.0882	1.0882
R(1,3)	1.0898	1.0913	1.0918	1.0918	1.0854	1.0899	1.0901	1.0901	1.089	1.0892	1.0878	1.0878	1.0878
R(1,4)	1.0933	1.0942	1.0945	1.0945	1.0889	1.0929	1.0931	1.0931	1.0925	1.0927	1.0912	1.0912	1.0912
R(1,10)	1.8818	1.8233	1.823	1.823	1.8812	1.8199	1.8204	1.8204	1.8149	1.815	1.811	1.8113	1.8114
R(5,6)	1.0933	1.0942	1.0945	1.0945	1.0889	1.0929	1.0931	1.0931	1.0925	1.0927	1.0912	1.0912	1.0912
R(5,7)	1.0903	1.0918	1.0922	1.0922	1.0861	1.0904	1.0906	1.0906	1.0895	1.0896	1.0882	1.0882	1.0882
R(5,8)	1.0898	1.0913	1.0918	1.0918	1.0854	1.0899	1.0901	1.0901	1.089	1.0892	1.0878	1.0878	1.0878
R(5,9)	1.8818	1.8233	1.823	1.823	1.8813	1.8199	1.8204	1.8204	1.8149	1.815	1.811	1.8113	1.8114
R(9,10)	2.2276	2.0637	2.0646	2.0647	2.2303	2.0732	2.0729	2.0727	2.0434	2.0435	2.0357	2.0359	2.0359
A(2,1,3)	110.8667	110.2419	110.2045	110.2062	110.8407	110.2469	110.2465	110.2868	110.4572	110.4486	110.4453	110.4422	110.4355
A(2,1,4)	109.8297	108.929	108.8862	108.8927	109.8318	108.9781	108.9661	108.9737	109.024	109.026	109.0145	109.0213	109.0253
A(2,1,10)	110.657	111.582	111.6507	111.6446	110.6997	111.5667	111.5643	111.5576	111.4318	111.4487	111.4536	111.4364	111.4418
A(3,1,4)	109.9898	109.2274	109.1756	109.1828	109.9618	109.2618	109.2533	109.2601	109.3302	109.3302	109.3358	109.3538	109.3541
A(3,1,10)	109.8438	110.7764	110.7891	110.7594	109.7792	110.686	110.7268	110.6775	110.5214	110.5706	110.5622	110.5711	110.5728
A(4,1,10)	105.5212	105.9573	106.0074	106.0294	105.5993	105.9788	105.9596	105.9604	105.9498	105.8877	105.9011	105.8881	105.8834
A(6,5,7)	109.8318	108.9279	108.8852	108.892	109.8318	108.9778	108.966	108.9737	109.0244	109.0263	109.0141	109.0208	109.0249
A(6,5,8)	109.9902	109.2285	109.1766	109.1836	109.9624	109.2627	109.254	109.2606	109.3311	109.3313	109.3359	109.354	109.3543
A(6,5,9)	105.5262	105.9551	106.0054	106.027	105.5989	105.9759	105.9568	105.9575	105.9464	105.8842	105.9008	105.8878	105.8831
A(7,5,8)	110.8679	110.242	110.2045	110.2063	110.841	110.247	110.2468	110.2871	110.4577	110.4492	110.4452	110.442	110.4354
A(7,5,9)	110.649	111.5832	111.6517	111.6462	110.7004	111.5683	111.5664	111.56	111.4343	111.4505	111.4543	111.4373	111.4427
A(8,5,9)	109.8434	110.7773	110.79	110.7599	109.778	110.6865	110.7266	110.6769	110.5204	110.5702	110.5621	110.5709	110.5727
A(5,9,10)	101.2458	103.5216	103.4902	103.4797	100.4999	102.7812	102.9788	102.9841	103.6586	103.82	104.006	103.9955	104.0054
A(1,10,9)	101.2513	103.5205	103.4894	103.4794	100.5009	102.7817	102.9797	102.9852	103.6599	103.8213	104.0055	103.9949	104.0048
D(2,1,10,9)	-65.3666	-65.5459	-65.663	-65.8244	-64.5698	-65.1578	-65.1594	-65.3513	-66.1716	-65.9356	-66.0145	-65.8292	-65.9052
D(3,1,10,9)	57.3686	57.6856	57.5784	57.3933	58.1172	58.004	58.0297	57.8493	57.0476	57.3195	57.2339	57.4094	57.3298
D(4,1,10,9)	175.8853	176.0334	175.9004	175.721	176.6116	176.3576	176.3834	176.1855	175.3789	175.6407	175.565	175.7592	175.6782
D(6,5,9,10)	175.8624	176.0221	175.8804	175.709	176.634	176.3196	176.3695	176.1918	175.4782	175.7222	175.5487	175.7499	175.6674
D(7,5,9,10)	-65.3883	-65.5592	-65.6848	-65.8378	-64.5473	-65.197	-65.174	-65.3454	-66.0725	-65.8549	-66.0311	-65.8387	-65.9163
D(8,5,9,10)	57.3427	57.6738	57.558	57.3815	58.1398	57.9665	58.0167	57.8569	57.1483	57.402	57.2176	57.4002	57.3191
D(5,9,10,1)	89.1781	87.4859	87.6888	87.543	90.2848	87.6992	87.9729	87.9326	87.1263	87.5838	87.3107	87.4975	87.4815
Energy	-876.003605662	-876.087324761	-876.090348205	-876.090494949	-876.073701833	-876.151935566	-876.154577926	-876.154954983	-876.172577588	-876.174644972	-876.178802454	-876.179601618	-876.179684899
ZPE Correction	0.078362	0.077915	0.077706	0.077697	0.07777	0.077413	0.077284	0.07729	0.07718	0.077117	0.077201	0.077174	0.077162

S8d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0972	1.098	1.0985	1.0985	1.0926	1.0963	1.0966	1.0965	1.0953	1.0955	1.0941	1.0941	1.0941
R(1,3)	1.0964	1.0974	1.098	1.098	1.0917	1.0957	1.096	1.096	1.0948	1.095	1.0936	1.0936	1.0936
R(1,4)	1.0998	1.1002	1.1006	1.1006	1.0953	1.0987	1.0989	1.0989	1.0981	1.0983	1.0967	1.0968	1.0968
R(1,10)	1.9141	1.8484	1.8486	1.8485	1.915	1.8445	1.8451	1.8451	1.8402	1.8404	1.835	1.8354	1.8354
R(5,6)	1.0998	1.1002	1.1006	1.1006	1.0953	1.0987	1.0989	1.0989	1.0981	1.0983	1.0967	1.0968	1.0968
R(5,7)	1.0972	1.0981	1.0985	1.0985	1.0926	1.0963	1.0966	1.0965	1.0953	1.0955	1.0941	1.0941	1.0941
R(5,8)	1.0964	1.0974	1.098	1.098	1.0916	1.0957	1.096	1.096	1.0948	1.095	1.0936	1.0936	1.0936
R(5,9)	1.9141	1.8484	1.8485	1.8485	1.915	1.8445	1.8451	1.8451	1.8402	1.8404	1.835	1.8354	1.8353
R(9,10)	2.2609	2.0845	2.0856	2.0857	2.2685	2.0975	2.0963	2.0961	2.062	2.0615	2.0516	2.0514	2.0516
A(2,1,3)	111.0734	110.3327	110.3061	110.299	111.1104	110.3795	110.371	110.4009	110.5273	110.5244	110.4911	110.4959	110.4879
A(2,1,4)	110.1929	109.2402	109.2036	109.2059	110.1965	109.2972	109.2803	109.286	109.3534	109.3583	109.3115	109.3331	109.3256
A(2,1,10)	110.1086	111.1114	111.1965	111.1897	110.1443	111.1208	111.1272	111.125	110.9633	110.9792	111.0017	110.9858	110.9912
A(3,1,4)	110.4402	109.6141	109.5612	109.5634	110.428	109.6482	109.629	109.6353	109.73	109.7261	109.7018	109.7256	109.7199
A(3,1,10)	109.4412	110.5007	110.5003	110.4769	109.3672	110.3876	110.4396	110.3927	110.2191	110.2725	110.3058	110.305	110.3145
A(4,1,10)	105.434	105.9358	105.967	106.0016	105.4417	105.9007	105.8856	105.8923	105.9398	105.8694	105.92	105.886	105.8926
A(6,5,7)	110.1913	109.2403	109.2041	109.2064	110.1957	109.2963	109.2794	109.2852	109.3532	109.3582	109.3125	109.3327	109.3266
A(6,5,8)	110.4434	109.6156	109.5623	109.5645	110.4299	109.649	109.6296	109.6359	109.7306	109.7266	109.7022	109.726	109.7203
A(6,5,9)	105.4344	105.9299	105.9617	105.9964	105.4414	105.9004	105.8853	105.8919	105.9388	105.8687	105.9187	105.8857	105.8909
A(7,5,8)	111.0744	110.3337	110.307	110.3	111.1106	110.3794	110.3709	110.4008	110.5275	110.5245	110.4916	110.496	110.4884
A(7,5,9)	110.1047	111.1154	111.2006	111.1935	110.142	111.1211	111.1273	111.1253	110.9637	110.9796	111.0009	110.9862	110.9911
A(8,5,9)	109.4422	110.4997	110.4988	110.4755	109.3685	110.3878	110.4402	110.3931	110.2191	110.2724	110.3062	110.3048	110.3144
A(5,9,10)	100.8116	103.4928	103.4755	103.4616	100.2449	102.8607	103.0599	103.0642	103.7528	103.9206	104.0949	104.1058	104.104
A(1,10,9)	100.8125	103.4962	103.4791	103.465	100.2447	102.8595	103.0586	103.063	103.753	103.9208	104.0956	104.106	104.1051
D(2,1,10,9)	-64.3887	-65.0318	-65.2481	-65.3584	-63.8721	-64.7604	-64.8049	-64.958	-65.7211	-65.5546	-65.6114	-65.3887	-65.5143
D(3,1,10,9)	57.9745	57.7891	57.5976	57.4572	58.5117	58.0476	58.0331	57.8837	57.0496	57.2603	57.1998	57.417	57.2916
D(4,1,10,9)	176.7677	176.4395	176.2029	176.0729	177.2571	176.6585	176.6398	176.477	175.6915	175.8852	175.8425	176.068	175.9446
D(6,5,9,10)	176.8043	176.475	176.2505	176.1341	177.2425	176.5872	176.5653	176.4086	175.6801	175.8728	175.8729	176.0517	175.9834
D(7,5,9,10)	-64.3557	-64.9976	-65.2009	-65.2976	-63.8891	-64.8328	-64.8807	-65.0275	-65.7331	-65.5674	-65.581	-65.4054	-65.4753
D(8,5,9,10)	58.0067	57.8267	57.6478	57.5208	58.4944	57.9755	57.9577	57.8146	57.038	57.2478	57.2303	57.4005	57.331
D(5,9,10,1)	86.0562	85.3817	85.6672	85.5036	86.8486	85.489	85.7652	85.7163	85.1426	85.5611	85.3517	85.5168	85.5503
Energy	-876.074829723	-876.149813135	-876.154043875	-876.154172681	-876.151011509	-876.22031191	-876.22259798	-876.222889516	-876.238378348	-876.240231639	-876.244768913	-876.245465498	-876.245529101
ZPE Correction	0.075651	0.075391	0.075158	0.075144	0.075075	0.074944	0.074817	0.074817	0.074768	0.074699	0.07482	0.074787	0.074776

S8e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0921	1.0933	1.0937	1.0937	1.0874	1.0916	1.0918	1.0917	1.0907	1.0909	1.0893	1.0893	1.0893
R(1,3)	1.0914	1.0925	1.0931	1.0931	1.0866	1.0909	1.0911	1.0911	1.0901	1.0903	1.0888	1.0888	1.0888
R(1,4)	1.0948	1.0955	1.0959	1.0959	1.0901	1.094	1.0942	1.0942	1.0937	1.0938	1.0922	1.0923	1.0923
R(1,10)	1.8958	1.8384	1.8382	1.8382	1.8955	1.8355	1.8358	1.8358	1.8287	1.8288	1.8251	1.8255	1.8255
R(5,6)	1.0948	1.0955	1.0959	1.0959	1.0901	1.094	1.0942	1.0942	1.0937	1.0938	1.0922	1.0923	1.0923
R(5,7)	1.0921	1.0933	1.0937	1.0937	1.0874	1.0916	1.0918	1.0917	1.0907	1.0909	1.0893	1.0893	1.0893
R(5,8)	1.0914	1.0925	1.0931	1.0931	1.0866	1.0909	1.0911	1.0911	1.0901	1.0903	1.0887	1.0888	1.0888
R(5,9)	1.8958	1.8384	1.8382	1.8382	1.8955	1.8355	1.8358	1.8358	1.8287	1.8288	1.8251	1.8255	1.8255
R(9,10)	2.2361	2.0828	2.0839	2.084	2.2399	2.0923	2.0917	2.0916	2.0619	2.0618	2.0556	2.0557	2.0558
A(2,1,3)	111.0213	110.3916	110.3623	110.3564	111.0166	110.4187	110.4149	110.4486	110.5852	110.576	110.5771	110.5748	110.5699
A(2,1,4)	110.054	109.1606	109.1117	109.1147	110.0541	109.2165	109.1936	109.2	109.2064	109.205	109.2116	109.2168	109.2204
A(2,1,10)	110.3523	111.2674	111.35	111.3444	110.3839	111.2453	111.25	111.2455	111.1544	111.173	111.1785	111.1641	111.1683
A(3,1,4)	110.2545	109.4969	109.4376	109.4417	110.2348	109.5397	109.5209	109.5281	109.5586	109.5532	109.567	109.581	109.5817
A(3,1,10)	109.5769	110.5241	110.5359	110.5121	109.4989	110.4168	110.4661	110.4173	110.3019	110.3536	110.3422	110.356	110.3559
A(4,1,10)	105.4374	105.8837	105.9263	105.9563	105.5112	105.8895	105.8795	105.8849	105.915	105.8583	105.8424	105.826	105.8227
A(6,5,7)	110.0555	109.1596	109.1109	109.114	110.0534	109.2166	109.1932	109.1997	109.2048	109.2033	109.2114	109.2166	109.2202
A(6,5,8)	110.2559	109.4981	109.4386	109.4426	110.2384	109.5399	109.5221	109.5292	109.5628	109.5573	109.5671	109.5811	109.5818
A(6,5,9)	105.4419	105.8809	105.9235	105.9534	105.5105	105.8891	105.8765	105.8819	105.9084	105.8515	105.8422	105.8259	105.8225
A(7,5,8)	111.0223	110.3917	110.3624	110.3566	111.0176	110.4188	110.4153	110.4489	110.5858	110.5768	110.577	110.5747	110.5698
A(7,5,9)	110.3442	111.268	111.3509	111.3456	110.379	111.2463	111.2505	111.246	111.1435	111.1615	111.1796	111.1653	111.1694
A(8,5,9)	109.5768	110.526	110.5373	110.5133	109.5006	110.4159	110.4672	110.4184	110.3159	110.3684	110.3415	110.3552	110.3551
A(5,9,10)	100.9697	103.1942	103.173	103.1584	100.2789	102.5028	102.6806	102.6822	103.2827	103.4333	103.6446	103.6409	103.648
A(1,10,9)	100.9752	103.1936	103.173	103.1587	100.2816	102.5029	102.6815	102.683	103.2821	103.4324	103.6443	103.6406	103.6477
D(2,1,10,9)	-64.9168	-65.1121	-65.3016	-65.4271	-64.1405	-64.7453	-64.7364	-64.9086	-65.5713	-65.4247	-65.6221	-65.4404	-65.5129
D(3,1,10,9)	57.6305	57.9093	57.7485	57.5947	58.3696	58.2196	58.2617	58.095	57.4624	57.6465	57.4463	57.6248	57.5489
D(4,1,10,9)	176.276	176.4021	176.2016	176.0576	176.9932	176.7103	176.7502	176.5694	175.9299	176.102	175.9032	176.0961	176.019
D(6,5,9,10)	176.2478	176.339	176.1453	176.0068	177.0453	176.7203	176.7257	176.5401	175.9435	176.0912	175.8978	176.0941	176.0162
D(7,5,9,10)	-64.9448	-65.1779	-65.3601	-65.4798	-64.0922	-64.735	-64.7628	-64.9398	-65.5693	-65.4477	-65.6273	-65.4421	-65.5154
D(8,5,9,10)	57.5982	57.8454	57.6918	57.5439	58.417	58.2301	58.2369	58.0655	57.4674	57.6269	57.4413	57.6233	57.5465
D(5,9,10,1)	88.2508	86.8175	87.0672	86.9067	89.3975	87.0147	87.2928	87.2266	86.6688	87.0834	86.7932	86.9779	86.9584
Energy	-875.997073939	-876.077254765	-876.080870007	-876.081005426	-876.066986743	-876.142220006	-876.144680887	-876.144996637	-876.162574039	-876.164485279	-876.168062177	-876.168826181	-876.16889178
ZPE Correction	0.077961	0.077545	0.077318	0.077309	0.077426	0.07706	0.076935	0.076938	0.07688	0.076812	0.076871	0.076845	0.076837

S8f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0914	1.0927	1.0932	1.0932	1.0866	1.091	1.0914	1.0914	1.0904	1.0907	1.0897	1.0897	1.0897
R(1,3)	1.0907	1.092	1.0927	1.0927	1.0858	1.0904	1.0908	1.0908	1.0898	1.0902	1.0892	1.0892	1.0892
R(1,4)	1.0942	1.0947	1.0953	1.0952	1.0896	1.0935	1.0938	1.0938	1.0933	1.0936	1.0924	1.0924	1.0924
R(1,10)	1.8822	1.8202	1.8201	1.8201	1.8817	1.8173	1.8177	1.8177	1.8144	1.8146	1.8086	1.8087	1.8087
R(5,6)	1.0942	1.0947	1.0953	1.0952	1.0896	1.0935	1.0938	1.0938	1.0933	1.0936	1.0924	1.0924	1.0924
R(5,7)	1.0914	1.0927	1.0932	1.0932	1.0866	1.091	1.0914	1.0914	1.0904	1.0907	1.0897	1.0897	1.0897
R(5,8)	1.0907	1.092	1.0927	1.0927	1.0858	1.0904	1.0908	1.0908	1.0898	1.0902	1.0892	1.0892	1.0892
R(5,9)	1.8822	1.8202	1.8201	1.8201	1.8817	1.8173	1.8177	1.8177	1.8144	1.8146	1.8086	1.8088	1.8087
R(9,10)	2.2306	2.05	2.0512	2.0513	2.2382	2.0629	2.0618	2.0617	2.0316	2.0311	2.0217	2.0216	2.0216
A(2,1,3)	110.8405	110.1605	110.1245	110.1167	110.9592	110.3171	110.2899	110.3023	110.4246	110.4231	110.3726	110.3662	110.3651
A(2,1,4)	109.7465	108.8051	108.75	108.7497	109.7746	108.9156	108.8749	108.8748	108.9574	108.952	108.9106	108.9053	108.9066
A(2,1,10)	110.8169	111.7728	111.8896	111.8826	110.8671	111.7644	111.7841	111.7811	111.5847	111.6071	111.6813	111.6844	111.6856
A(3,1,4)	109.9318	109.1277	109.0592	109.0571	109.9281	109.2102	109.1796	109.187	109.2885	109.2823	109.2496	109.25	109.2509
A(3,1,10)	110.0894	111.1009	111.1105	111.0974	110.0092	110.9449	111.0091	110.9809	110.7687	110.8173	110.8823	110.9014	110.9007
A(4,1,10)	105.2727	105.7276	105.7569	105.7892	105.1467	105.5362	105.5491	105.5611	105.6735	105.6119	105.5949	105.5835	105.5819
A(6,5,7)	109.7461	108.805	108.75	108.7497	109.7737	108.9156	108.8749	108.8748	108.9574	108.9519	108.9112	108.9057	108.9069
A(6,5,8)	109.9329	109.1273	109.0588	109.0567	109.9311	109.2101	109.1795	109.1869	109.2882	109.2822	109.2488	109.2493	109.2503
A(6,5,9)	105.2726	105.7276	105.7569	105.789	105.1468	105.5355	105.5484	105.5604	105.6735	105.612	105.5955	105.5841	105.5825
A(7,5,8)	110.8411	110.1601	110.1242	110.1164	110.9603	110.317	110.2898	110.3022	110.4245	110.4229	110.3725	110.3661	110.365
A(7,5,9)	110.8153	111.7748	111.8913	111.8844	110.8613	111.7656	111.7855	111.7825	111.5856	111.6076	111.6818	111.6845	111.6857
A(8,5,9)	110.0897	111.0996	111.1095	111.0964	110.0118	110.9446	111.0086	110.9804	110.7681	110.8171	110.8816	110.9011	110.9005
A(5,9,10)	102.02	104.5409	104.5381	104.5259	101.6849	104.0901	104.2227	104.2264	104.7251	104.8724	105.0912	105.0934	105.0975
A(1,10,9)	102.0206	104.5411	104.5385	104.5264	101.6853	104.0909	104.2234	104.2271	104.7254	104.8726	105.0917	105.0937	105.0977
D(2,1,10,9)	-65.1558	-65.498	-65.7486	-65.8123	-64.692	-65.3576	-65.4068	-65.4862	-65.9294	-65.8423	-65.9262	-65.8167	-65.8685
D(3,1,10,9)	57.8228	58.0015	57.7963	57.7076	58.4162	58.2247	58.2016	58.1154	57.5343	57.6708	57.6222	57.7396	57.6868
D(4,1,10,9)	176.2565	176.2668	176.0021	175.923	176.7342	176.3944	176.3758	176.2908	175.7853	175.9039	175.8405	175.9616	175.9086
D(6,5,9,10)	176.2582	176.2541	175.9829	175.9044	176.7407	176.36	176.3497	176.2655	175.7828	175.8958	175.829	175.9438	175.8908
D(7,5,9,10)	-65.1554	-65.5096	-65.7669	-65.8301	-64.6895	-65.3918	-65.4326	-65.5112	-65.9313	-65.8502	-65.9364	-65.8336	-65.8855
D(8,5,9,10)	57.8231	57.99	57.7781	57.6901	58.4178	58.1911	58.1763	58.091	57.5324	57.6628	57.6117	57.7224	57.6695
D(5,9,10,1)	87.8981	86.6978	87.0588	86.9436	89.4682	87.3442	87.4287	87.3768	86.9551	87.1944	87.0045	87.1246	87.0947
Energy	-876.216748308	-876.298125183	-876.303173049	-876.303304398	-876.289971053	-876.365928692	-876.368132855	-876.36837215	-876.385174186	-876.386856325	-876.390556691	-876.391193117	-876.391231657
ZPE Correction	0.077627	0.07722	0.076956	0.076942	0.077133	0.0768	0.076643	0.076639	0.076486	0.076383	0.076461	0.076443	0.076435

S8g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0904	1.0916	1.0921	1.0921	1.0859	1.0901	1.0906	1.0905	1.0895	1.0898	1.0886	1.0886	1.0887
R(1,3)	1.0898	1.0911	1.0917	1.0917	1.0852	1.0896	1.0901	1.0901	1.089	1.0894	1.0882	1.0883	1.0883
R(1,4)	1.0933	1.0941	1.0945	1.0945	1.0889	1.0929	1.0932	1.0932	1.0927	1.093	1.0917	1.0918	1.0918
R(1,10)	1.8859	1.826	1.8257	1.8256	1.8854	1.823	1.8234	1.8234	1.8187	1.8188	1.814	1.8143	1.8143
R(5,6)	1.0933	1.0941	1.0945	1.0945	1.0888	1.0929	1.0932	1.0932	1.0927	1.093	1.0917	1.0918	1.0918
R(5,7)	1.0903	1.0917	1.0921	1.0921	1.0859	1.0902	1.0906	1.0905	1.0895	1.0898	1.0886	1.0887	1.0887
R(5,8)	1.0898	1.0911	1.0917	1.0917	1.0852	1.0896	1.0901	1.0901	1.089	1.0894	1.0882	1.0882	1.0883
R(5,9)	1.8859	1.826	1.8257	1.8256	1.8854	1.823	1.8234	1.8234	1.8187	1.8188	1.814	1.8143	1.8143
R(9,10)	2.2302	2.0618	2.0628	2.0628	2.2344	2.0727	2.0718	2.0717	2.0422	2.0418	2.0343	2.0341	2.0341
A(2,1,3)	110.913	110.2492	110.2104	110.2144	110.9826	110.3619	110.3339	110.3569	110.4993	110.4939	110.4616	110.4589	110.4545
A(2,1,4)	109.8518	108.9176	108.8661	108.87	109.8833	109.0199	108.9872	108.9901	109.0394	109.0398	109.0076	109.0098	109.011
A(2,1,10)	110.7298	111.7061	111.8097	111.8033	110.7716	111.6832	111.7053	111.6988	111.5401	111.5678	111.6117	111.6083	111.6121
A(3,1,4)	109.9911	109.1893	109.1247	109.1273	109.9958	109.2714	109.2449	109.2511	109.326	109.3224	109.3015	109.3088	109.3095
A(3,1,10)	109.952	110.9484	110.9599	110.9376	109.8724	110.8117	110.8679	110.8353	110.6607	110.7063	110.7348	110.7478	110.7504
A(4,1,10)	105.2567	105.6872	105.7246	105.744	105.181	105.5463	105.5543	105.5613	105.6315	105.5634	105.5761	105.5595	105.5555
A(6,5,7)	109.851	108.9171	108.8659	108.87	109.8811	109.0205	108.9875	108.9905	109.0396	109.0399	109.0079	109.0102	109.0114
A(6,5,8)	109.9943	109.1898	109.125	109.1275	110.0009	109.2717	109.2451	109.2513	109.3263	109.3227	109.3018	109.309	109.3097
A(6,5,9)	105.2585	105.6851	105.7226	105.7419	105.1813	105.5436	105.5518	105.5587	105.6301	105.5623	105.5752	105.5585	105.5546
A(7,5,8)	110.9141	110.2492	110.2105	110.2145	110.9831	110.3621	110.3342	110.3571	110.4995	110.4941	110.4619	110.4592	110.4548
A(7,5,9)	110.7229	111.7075	111.8112	111.8051	110.7638	111.6847	111.7067	111.7003	111.5402	111.5676	111.6113	111.6082	111.6119
A(8,5,9)	109.9536	110.9489	110.9601	110.9375	109.8766	110.8118	110.868	110.8353	110.6614	110.707	110.7352	110.7479	110.7506
A(5,9,10)	101.9312	104.2895	104.2729	104.2682	101.5104	103.7843	103.9204	103.9231	104.4465	104.5989	104.7914	104.7927	104.8005
A(1,10,9)	101.9337	104.2894	104.2733	104.2689	101.511	103.7853	103.9213	103.9242	104.4465	104.5988	104.7915	104.793	104.8007
D(2,1,10,9)	-65.4013	-65.7516	-66.0042	-66.1418	-64.9136	-65.6259	-65.6432	-65.7429	-66.3057	-66.181	-66.291	-66.176	-66.2233
D(3,1,10,9)	57.5154	57.7032	57.4835	57.33	58.065	57.8586	57.8619	57.7635	57.1445	57.3149	57.2153	57.3336	57.2854
D(4,1,10,9)	175.9404	175.938	175.6692	175.5186	176.4129	176.0379	176.0434	175.9395	175.3594	175.5099	175.4077	175.5317	175.4833
D(6,5,9,10)	175.9302	175.8886	175.6185	175.4759	176.4166	176.0344	176.0285	175.9319	175.3547	175.5048	175.4133	175.5439	175.4922
D(7,5,9,10)	-65.4149	-65.8021	-66.0556	-66.1849	-64.9164	-65.6295	-65.6584	-65.7506	-66.311	-66.1867	-66.2857	-66.1639	-66.2146
D(8,5,9,10)	57.4997	57.6541	57.4334	57.2884	58.0604	57.8563	57.8481	57.7571	57.1398	57.3098	57.221	57.3461	57.2945
D(5,9,10,1)	89.171	87.6708	88.04	87.9015	90.5611	88.1558	88.3579	88.329	87.6126	87.9529	87.7322	87.891	87.867
Energy	-876.059870264	-876.141036791	-876.145685227	-876.145811124	-876.129684677	-876.206390684	-876.208766507	-876.20904639	-876.226651282	-876.228525099	-876.231580758	-876.232244976	-876.23229949
ZPE Correction	0.078183	0.077725	0.077475	0.077457	0.077649	0.077268	0.077107	0.077102	0.076975	0.076875	0.076933	0.076903	0.076891

S8h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0986	1.0996	1.1002	1.1002	1.094	1.0978	1.0981	1.0981	1.097	1.0972	1.0958	1.0958	1.0958
R(1,3)	1.098	1.099	1.0997	1.0997	1.0932	1.0972	1.0975	1.0975	1.0964	1.0967	1.0953	1.0953	1.0953
R(1,4)	1.1016	1.102	1.1025	1.1025	1.0971	1.1005	1.1007	1.1007	1.1001	1.1003	1.0988	1.0989	1.0989
R(1,10)	1.8963	1.8366	1.8365	1.8364	1.8968	1.8329	1.8334	1.8334	1.828	1.8282	1.8237	1.824	1.824
R(5,6)	1.1016	1.102	1.1025	1.1025	1.097	1.1005	1.1007	1.1007	1.1001	1.1003	1.0988	1.0989	1.0989
R(5,7)	1.0986	1.0996	1.1002	1.1002	1.094	1.0978	1.0981	1.0981	1.097	1.0972	1.0958	1.0958	1.0958
R(5,8)	1.0979	1.099	1.0997	1.0997	1.0932	1.0972	1.0975	1.0975	1.0964	1.0967	1.0953	1.0953	1.0953
R(5,9)	1.8963	1.8366	1.8365	1.8364	1.8969	1.8329	1.8334	1.8334	1.828	1.8281	1.8237	1.824	1.824
R(9,10)	2.2446	2.0771	2.078	2.0781	2.2506	2.0881	2.087	2.0868	2.0548	2.0544	2.0465	2.0464	2.0464
A(2,1,3)	111.0086	110.3625	110.3106	110.2996	111.0182	110.3777	110.3674	110.4015	110.5836	110.5786	110.5718	110.5719	110.5666
A(2,1,4)	109.9032	108.9904	108.9208	108.9236	109.8852	109.019	108.9927	109.0007	109.0994	109.0963	109.0876	109.0917	109.0958
A(2,1,10)	110.593	111.5025	111.6304	111.6233	110.6474	111.5186	111.5337	111.5295	111.3453	111.3706	111.3695	111.3576	111.3622
A(3,1,4)	110.085	109.3162	109.2311	109.2332	110.0455	109.336	109.3128	109.3209	109.4374	109.4301	109.4359	109.4493	109.4502
A(3,1,10)	109.7757	110.7382	110.7605	110.7366	109.7034	110.6376	110.6949	110.6405	110.4303	110.4857	110.4746	110.4884	110.4887
A(4,1,10)	105.327	105.7987	105.8531	105.8928	105.3946	105.8222	105.8071	105.8154	105.8136	105.7447	105.7681	105.7481	105.7436
A(6,5,7)	109.902	108.9901	108.9193	108.9224	109.8821	109.0185	108.9923	109.0003	109.0989	109.0957	109.0873	109.0911	109.0952
A(6,5,8)	110.0885	109.3163	109.2328	109.2347	110.0516	109.3379	109.3145	109.3225	109.4396	109.4322	109.4381	109.4518	109.4527
A(6,5,9)	105.3291	105.7987	105.8488	105.8881	105.395	105.8173	105.8022	105.8104	105.8085	105.7396	105.7634	105.743	105.7385
A(7,5,8)	111.0095	110.3623	110.3111	110.3002	111.0186	110.3784	110.3683	110.4024	110.5844	110.5796	110.5726	110.5728	110.5675
A(7,5,9)	110.5863	111.5038	111.6313	111.6247	110.6382	111.5194	111.5349	111.5309	111.3458	111.3702	111.3694	111.3567	111.3613
A(8,5,9)	109.7772	110.7372	110.7631	110.7388	109.709	110.6393	110.6963	110.6419	110.4323	110.4885	110.4764	110.4915	110.4917
A(5,9,10)	101.198	103.6585	103.6479	103.6282	100.493	102.8895	103.1031	103.1064	103.7432	103.9187	104.1038	104.1025	104.1106
A(1,10,9)	101.2011	103.6575	103.6483	103.629	100.4935	102.891	103.1051	103.1084	103.7444	103.9197	104.1052	104.1038	104.1119
D(2,1,10,9)	-65.3053	-65.5251	-65.7975	-65.9296	-64.5414	-65.1847	-65.3397	-65.5008	-66.2002	-66.0834	-66.1794	-65.9827	-66.0536
D(3,1,10,9)	57.5197	57.7777	57.5457	57.3769	58.2831	58.0767	57.9605	57.8012	57.0554	57.223	57.1095	57.3079	57.2336
D(4,1,10,9)	176.0053	176.1186	175.8286	175.6728	176.7231	176.4019	176.2795	176.1061	175.3877	175.536	175.4369	175.647	175.5714
D(6,5,9,10)	176.0111	176.1203	175.7385	175.5957	176.7362	176.3711	176.2674	176.0962	175.4557	175.5893	175.5136	175.7064	175.6313
D(7,5,9,10)	-65.3031	-65.523	-65.8916	-66.0103	-64.5366	-65.2187	-65.3547	-65.5134	-66.1357	-66.034	-66.106	-65.9276	-65.998
D(8,5,9,10)	57.5195	57.7797	57.4547	57.2995	58.2859	58.0455	57.9485	57.7916	57.1227	57.2754	57.1853	57.3657	57.292
D(5,9,10,1)	87.9739	86.7085	87.0302	86.8504	89.0602	86.9825	87.2199	87.1626	86.6049	87.0163	86.7881	86.969	86.9439
Energy	-875.643095249	-875.720524056	-875.72541056	-875.72557294	-875.718349602	-875.78944571	-875.79187847	-875.792185427	-875.80952988	-875.811456129	-875.815503082	-875.816238222	-875.81630107
ZPE Correction	0.076146	0.0757	0.075443	0.07543	0.075574	0.075221	0.07507	0.075069	0.074999	0.074912	0.07501	0.074976	0.074966

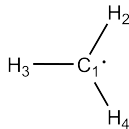
S8i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0926	1.0938	1.0942	1.0942	1.0878	1.0918	1.0921	1.092	1.0909	1.091	1.0894	1.0894	1.0894
R(1,3)	1.0919	1.0931	1.0936	1.0936	1.087	1.0912	1.0915	1.0915	1.0903	1.0905	1.0889	1.0889	1.0889
R(1,4)	1.0954	1.096	1.0964	1.0964	1.0906	1.0944	1.0945	1.0945	1.0939	1.094	1.0923	1.0924	1.0924
R(1,10)	1.8937	1.8361	1.8358	1.8358	1.8926	1.8325	1.833	1.8329	1.8257	1.8257	1.8221	1.8226	1.8226
R(5,6)	1.0954	1.096	1.0964	1.0964	1.0906	1.0944	1.0945	1.0945	1.0939	1.094	1.0923	1.0924	1.0924
R(5,7)	1.0926	1.0938	1.0942	1.0942	1.0878	1.0918	1.0921	1.092	1.0909	1.0911	1.0894	1.0894	1.0894
R(5,8)	1.092	1.0931	1.0936	1.0936	1.087	1.0912	1.0915	1.0914	1.0903	1.0905	1.0889	1.0889	1.0889
R(5,9)	1.8937	1.8361	1.8358	1.8358	1.8927	1.8325	1.8329	1.8329	1.8256	1.8257	1.8221	1.8226	1.8226
R(9,10)	2.2348	2.0779	2.0787	2.0788	2.2395	2.0864	2.086	2.0858	2.056	2.0559	2.0492	2.0494	2.0494
A(2,1,3)	111.0068	110.3813	110.3478	110.3439	111.007	110.4087	110.4085	110.4457	110.5775	110.5698	110.571	110.5713	110.5656
A(2,1,4)	110.0154	109.1265	109.0805	109.0845	110.0138	109.1827	109.1684	109.1751	109.195	109.1957	109.1869	109.1963	109.2006
A(2,1,10)	110.4445	111.3608	111.4376	111.4315	110.4803	111.3391	111.3352	111.3307	111.2378	111.2518	111.2506	111.2319	111.2364
A(3,1,4)	110.1908	109.4334	109.3781	109.3836	110.163	109.4706	109.4624	109.4689	109.5137	109.5135	109.52	109.539	109.5398
A(3,1,10)	109.6474	110.5602	110.5733	110.5478	109.5647	110.4492	110.4926	110.4421	110.3244	110.373	110.3599	110.3681	110.3681
A(4,1,10)	105.3908	105.8579	105.9026	105.9303	105.4698	105.8725	105.8541	105.858	105.8695	105.8116	105.8277	105.8097	105.8059
A(6,5,7)	110.0178	109.1254	109.0797	109.0839	110.0122	109.1829	109.1685	109.1753	109.1951	109.1959	109.1867	109.1961	109.2004
A(6,5,8)	110.1911	109.4347	109.3792	109.3845	110.1669	109.4719	109.4635	109.4698	109.5153	109.5152	109.5202	109.5391	109.5399
A(6,5,9)	105.3961	105.8548	105.8993	105.9267	105.4699	105.868	105.8495	105.8534	105.8649	105.8066	105.8271	105.809	105.8053
A(7,5,8)	111.0076	110.3812	110.3478	110.3439	111.0073	110.4091	110.4091	110.4461	110.578	110.5704	110.571	110.5712	110.5655
A(7,5,9)	110.4367	111.3616	111.4388	111.4333	110.4744	111.3413	111.3382	111.3338	111.2398	111.2532	111.252	111.2335	111.2379
A(8,5,9)	109.6466	110.5623	110.575	110.5491	109.5679	110.4494	110.4924	110.4419	110.3247	110.3741	110.3593	110.3673	110.3674
A(5,9,10)	101.1064	103.334	103.3089	103.2979	100.3988	102.6463	102.8412	102.8451	103.5061	103.6596	103.8315	103.8261	103.8346
A(1,10,9)	101.1126	103.3319	103.3077	103.2973	100.4002	102.6476	102.843	102.8468	103.5069	103.6603	103.8309	103.8256	103.8341
D(2,1,10,9)	-65.0581	-65.3881	-65.5351	-65.6871	-64.363	-65.0854	-65.1183	-65.2966	-66.021	-65.8097	-65.9436	-65.7491	-65.8289
D(3,1,10,9)	57.579	57.7113	57.5846	57.4051	58.2426	57.955	57.95	57.7803	57.0767	57.3222	57.1797	57.3673	57.2833
D(4,1,10,9)	176.1595	176.1326	175.9728	175.8025	176.7922	176.3707	176.3681	176.1818	175.4764	175.7138	175.5815	175.7855	175.7004
D(6,5,9,10)	176.1274	176.0706	175.9085	175.7417	176.8084	176.3761	176.3728	176.1836	175.5395	175.7572	175.5833	175.7922	175.7056
D(7,5,9,10)	-65.0884	-65.4528	-65.6017	-65.7499	-64.3517	-65.0813	-65.1146	-65.2957	-65.9594	-65.7684	-65.9418	-65.7423	-65.8236
D(8,5,9,10)	57.5441	57.6484	57.5199	57.3445	58.2525	57.9614	57.9562	57.7838	57.1404	57.3659	57.1819	57.3745	57.2891
D(5,9,10,1)	88.7525	87.2964	87.5347	87.3682	89.7696	87.5412	87.758	87.7032	86.9488	87.3569	87.147	87.3426	87.3208
Energy	-876.032265467	-876.112184364	-876.115587861	-876.115722561	-876.105689682	-876.179614106	-876.18213385	-876.182470744	-876.199471748	-876.201474228	-876.206041278	-876.20680881	-876.206879251
ZPE Correction	0.077635	0.077218	0.077008	0.076998	0.0771	0.076773	0.076644	0.076647	0.076591	0.076522	0.076595	0.076567	0.076557

S8j – QCISD

	QCISD/cc-pVTZ
R(1,2)	1.0875
R(1,3)	1.0866
R(1,4)	1.0899
R(1,10)	1.8187
R(5,6)	1.0899
R(5,7)	1.0875
R(5,8)	1.0866
R(5,9)	1.8187
R(9,10)	2.0585
A(2,1,3)	110.2665
A(2,1,4)	109.1252
A(2,1,10)	110.9657
A(3,1,4)	109.5877
A(3,1,10)	110.3446
A(4,1,10)	106.4655
A(6,5,7)	109.1253
A(6,5,8)	109.5879
A(6,5,9)	106.4654
A(7,5,8)	110.2666
A(7,5,9)	110.966
A(8,5,9)	110.344
A(5,9,10)	102.0479
A(1,10,9)	102.0478
D(2,1,10,9)	-63.4004
D(3,1,10,9)	59.1272
D(4,1,10,9)	177.9718
D(6,5,9,10)	177.9799
D(7,5,9,10)	-63.3921
D(8,5,9,10)	59.1354
D(5,9,10,1)	85.7054
Energy	-875.117806
ZPE Correction	0.077833

S9 – Me·



S9a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0834	1.0824	1.0831	1.0831	1.0796	1.0806	1.0808	1.0808	1.0794	1.0796	1.078	1.078	1.078
R(1,3)	1.0834	1.0824	1.0831	1.0831	1.0796	1.0806	1.0808	1.0808	1.0794	1.0796	1.078	1.078	1.078
R(1,4)	1.0834	1.0824	1.0831	1.0831	1.0796	1.0806	1.0808	1.0808	1.0794	1.0796	1.078	1.078	1.078
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	180	180	180	180	180	180	180	180	180	180
Energy	-39.8311735205	-39.8428796083	-39.8473342517	-39.8473761053	-39.8417923092	-39.8537574964	-39.855166594	-39.8551878191	-39.8551168079	-39.8565465345	-39.8570783988	-39.8583317168	-39.8583566953
ZPE Correction	0.030046	0.029745	0.029803	0.029804	0.029738	0.02957	0.029636	0.029633	0.02961	0.029679	0.029636	0.029711	0.02971

S9b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0826	1.0819	1.0825	1.0825	1.0797	1.0807	1.0808	1.0809	1.0796	1.0797	1.0782	1.0783	1.0783
R(1,3)	1.0826	1.0819	1.0825	1.0825	1.0797	1.0807	1.0808	1.0809	1.0796	1.0797	1.0782	1.0783	1.0783
R(1,4)	1.0826	1.0819	1.0825	1.0825	1.0797	1.0807	1.0808	1.0809	1.0796	1.0797	1.0782	1.0783	1.0783
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	180	180	180	180	180	180	180	180	180	180
Energy	-39.9924560529	-40.003882352	-40.0072032446	-40.007249712	-40.0017385119	-40.0136903294	-40.0147359968	-40.0147692141	-40.015015505	-40.0160782642	-40.0167424288	-40.0176479815	-40.0176821626
ZPE Correction	0.030173	0.029856	0.029909	0.029909	0.029841	0.029664	0.029716	0.029713	0.029697	0.029751	0.029713	0.029768	0.029767

S9c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0833	1.0827	1.0832	1.0832	1.0805	1.0815	1.0817	1.0817	1.0805	1.0806	1.0792	1.0792	1.0792
R(1,3)	1.0833	1.0827	1.0832	1.0832	1.0805	1.0815	1.0817	1.0817	1.0805	1.0806	1.0792	1.0792	1.0792
R(1,4)	1.0833	1.0827	1.0832	1.0832	1.0805	1.0815	1.0817	1.0817	1.0805	1.0806	1.0792	1.0792	1.0792
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	-180	180	180	180	-180	180	-180	-180	180	180	180
Energy	-39.8161905387	-39.8275177566	-39.8309673862	-39.8310203289	-39.8251993857	-39.8370984538	-39.8382435909	-39.8382811885	-39.8383910021	-39.8395586698	-39.8400749021	-39.8410532135	-39.8410900653
ZPE Correction	0.030117	0.029801	0.029862	0.029861	0.029785	0.029603	0.02966	0.029655	0.029632	0.029691	0.029645	0.029705	0.029704

S9d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.09	1.0886	1.0892	1.0892	1.0862	1.0868	1.087	1.087	1.0856	1.0858	1.0845	1.0845	1.0845
R(1,3)	1.09	1.0886	1.0892	1.0892	1.0862	1.0868	1.087	1.087	1.0856	1.0858	1.0845	1.0845	1.0845
R(1,4)	1.09	1.0886	1.0892	1.0892	1.0862	1.0868	1.087	1.087	1.0856	1.0858	1.0845	1.0845	1.0845
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	180	180	180	180	180	180	-180	180	180	180
Energy	-39.8028103677	-39.8138341096	-39.8177094494	-39.8177487362	-39.8123085505	-39.8238392646	-39.8250684083	-39.8250942349	-39.8251206565	-39.8263776215	-39.8270716361	-39.8280791148	-39.828119694
ZPE Correction	0.029369	0.029147	0.029177	0.029177	0.029027	0.028955	0.028997	0.028993	0.028988	0.029033	0.029013	0.029063	0.029062

S9e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0854	1.0843	1.0849	1.0849	1.0816	1.0826	1.0827	1.0827	1.0815	1.0816	1.0802	1.0801	1.0802
R(1,3)	1.0854	1.0843	1.0849	1.0849	1.0816	1.0826	1.0827	1.0827	1.0815	1.0816	1.0802	1.0801	1.0802
R(1,4)	1.0854	1.0843	1.0849	1.0849	1.0816	1.0826	1.0827	1.0827	1.0815	1.0816	1.0802	1.0801	1.0802
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	-180	180	-180	180	180	180	180	180	-180	180
Energy	-39.809921001	-39.8210631716	-39.8248745142	-39.8249095665	-39.819122739	-39.8308878132	-39.8321642817	-39.8321909511	-39.8321093188	-39.8334050402	-39.8338403336	-39.8349602645	-39.8349932298
ZPE Correction	0.029969	0.029682	0.029742	0.029742	0.029651	0.029489	0.029551	0.029548	0.029521	0.029586	0.029539	0.029608	0.029608

S9f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0847	1.0835	1.0843	1.0842	1.081	1.0821	1.0825	1.0825	1.0812	1.0815	1.0804	1.0804	1.0804
R(1,3)	1.0847	1.0835	1.0843	1.0842	1.081	1.0821	1.0825	1.0825	1.0812	1.0815	1.0804	1.0804	1.0804
R(1,4)	1.0847	1.0835	1.0843	1.0842	1.081	1.0821	1.0825	1.0825	1.0812	1.0815	1.0804	1.0804	1.0804
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	180	180	180	180	180	180	180	180	-180	180
Energy	-39.8379507347	-39.8493353972	-39.8535351669	-39.8536000317	-39.8467934081	-39.8589727551	-39.8603154866	-39.8603444684	-39.8599252726	-39.8612861026	-39.8617945507	-39.862887216	-39.8629051079
ZPE Correction	0.029762	0.029478	0.029512	0.029517	0.029419	0.029243	0.029281	0.029282	0.029271	0.029309	0.029276	0.029337	0.029316

S9g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0836	1.0827	1.0833	1.0833	1.0804	1.0816	1.0818	1.0819	1.0806	1.0809	1.0798	1.0798	1.0798
R(1,3)	1.0836	1.0827	1.0833	1.0833	1.0804	1.0816	1.0818	1.0819	1.0806	1.0809	1.0798	1.0798	1.0798
R(1,4)	1.0836	1.0827	1.0833	1.0833	1.0804	1.0816	1.0818	1.0819	1.0806	1.0809	1.0798	1.0798	1.0798
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	180	180	180	180	180	180	180	180	180	180
Energy	-39.8144480722	-39.8254630326	-39.8301305348	-39.8301701991	-39.8235491946	-39.8354288131	-39.8371710612	-39.8371850606	-39.8364639746	-39.8382328813	-39.838124718	-39.8395681134	-39.8395904638
ZPE Correction	0.030001	0.029683	0.029749	0.029746	0.029685	0.029466	0.029533	0.029527	0.029478	0.029547	0.029478	0.029562	0.029561

S9h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0909	1.0898	1.0906	1.0906	1.0873	1.0881	1.0884	1.0884	1.0872	1.0875	1.0861	1.0861	1.0862
R(1,3)	1.0909	1.0898	1.0906	1.0906	1.0873	1.0881	1.0884	1.0884	1.0872	1.0875	1.0861	1.0861	1.0862
R(1,4)	1.0909	1.0898	1.0906	1.0906	1.0873	1.0881	1.0884	1.0884	1.0872	1.0875	1.0861	1.0861	1.0862
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	180	180	180	-180	180	180	180	180	180	180	180	180	180
Energy	-39.7621860975	-39.7726064368	-39.7774183836	-39.7774638056	-39.7721712225	-39.7830867148	-39.7847531811	-39.7847760779	-39.7842762104	-39.785968258	-39.7860842126	-39.7875148569	-39.7875411788
ZPE Correction	0.029448	0.02915	0.029199	0.029199	0.029145	0.028962	0.029025	0.029021	0.028986	0.029052	0.029003	0.029076	0.029074

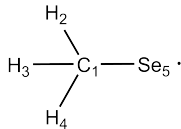
S9i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0858	1.0847	1.0852	1.0852	1.082	1.0828	1.0829	1.0829	1.0816	1.0817	1.0802	1.0802	1.0802
R(1,3)	1.0858	1.0847	1.0852	1.0852	1.082	1.0828	1.0829	1.0829	1.0816	1.0817	1.0802	1.0802	1.0802
R(1,4)	1.0858	1.0847	1.0852	1.0852	1.082	1.0828	1.0829	1.0829	1.0816	1.0817	1.0802	1.0802	1.0802
A(2,1,3)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(2,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
A(3,1,4)	120	120	120	120	120	120	120	120	120	120	120	120	120
D(2,1,4,3)	-180	180	180	180	180	180	180	180	-180	180	180	-180	180
Energy	-39.825978892	-39.836922014	-39.8403929924	-39.8404268246	-39.8352356845	-39.8465919395	-39.8477194903	-39.8477552617	-39.847924976	-39.8490754739	-39.84985889	-39.8508163536	-39.8508605408
ZPE Correction	0.029861	0.029595	0.029644	0.029644	0.029535	0.029407	0.029457	0.029453	0.029447	0.0295	0.029471	0.029526	0.029526

S9j – QCISD/cc-pVTZ

	QCISD/cc-pVTZ
R(1,2)	1.0779
R(1,3)	1.0779
R(1,4)	1.0779
A(2,1,3)	120
A(2,1,4)	120
A(3,1,4)	120
D(2,1,4,3)	180
Energy	-39.7564011
ZPE Correction	0.029891

S10 – MeSe.



S10a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0898	1.0947	1.0917	1.0962	1.0911	1.0934	1.089	1.0886	1.0874	1.0876	1.0858	1.0859	1.0859
R(1,3)	1.0945	1.0901	1.0962	1.0912	1.0859	1.0886	1.0933	1.0935	1.0923	1.0877	1.0907	1.0906	1.0907
R(1,4)	1.089	1.0901	1.0908	1.0912	1.0859	1.0886	1.0884	1.0886	1.0874	1.0924	1.0858	1.0856	1.0856
R(1,5)	1.99	1.9552	1.9456	1.9479	1.9814	1.9607	1.9606	1.9607	1.9539	1.9528	1.9525	1.9527	1.9527
A(2,1,3)	109.2862	108.9921	108.3112	108.7296	108.8628	108.9609	108.7262	108.9719	108.8929	111.3445	108.947	108.8858	108.8706
A(2,1,4)	111.7572	108.9933	111.0798	108.7258	108.8594	108.9615	111.386	111.4374	111.3263	108.9471	111.4177	111.4244	111.4294
A(2,1,5)	109.5663	106.1716	110.5697	106.3801	107.0737	106.3213	110.1529	110.5193	110.6478	110.6264	110.5958	110.4176	110.4053
A(3,1,4)	109.7521	111.4638	108.8443	111.3422	111.1442	111.4217	109.2324	108.9543	108.881	108.902	108.929	109.0595	109.0747
A(3,1,5)	106.2211	110.5261	106.7458	110.7484	110.3974	110.5086	106.4253	106.2931	106.3096	110.5146	106.2174	106.2715	106.2594
A(4,1,5)	110.1013	110.5298	111.1364	110.7477	110.3903	110.5109	110.7678	110.5067	110.6248	106.3523	110.5704	110.6236	110.6418
D(2,1,4,3)	-121.4103	-120.3416	-119.1656	-119.7663	-119.8952	-120.2555	-120.1184	-120.2744	-120.0591	-121.6218	-120.2145	-120.2279	-120.2222
D(2,1,5,3)	117.9346	118.0595	117.6033	117.9858	118.362	118.0998	117.6923	118.1023	118.086	123.785	118.0693	117.9333	117.9018
D(2,1,5,4)	-123.2973	-118.0629	-123.8449	-117.9809	-118.354	-118.1018	-123.6828	-123.823	-123.8545	-118.1643	-123.8963	-123.8169	-123.8275
D(3,1,5,4)	118.768	123.8777	118.5518	124.0334	123.284	123.7984	118.6249	118.0746	118.0595	118.0508	118.0344	118.2498	118.2706
Energy	-2439.02888346	-2439.25777375	-2439.27926751	-2439.27996089	-2441.41042604	-2441.44410141	-2441.44474388	-2441.44480388	-2441.44553382	-2441.44620510	-2441.45098112	-2441.45148043	-2441.45150524
ZPE Correction	0.035613	0.035286	0.035321	0.03516	0.035171	0.034959	0.034887	0.034821	0.035044	0.034913	0.03508	0.034979	0.034923

S10b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0942	1.09	1.091	1.091	1.0915	1.0889	1.0937	1.0937	1.0927	1.0928	1.0913	1.0913	1.0913
R(1,3)	1.089	1.0945	1.0959	1.0959	1.0861	1.0937	1.0889	1.0888	1.0879	1.088	1.0864	1.0863	1.0863
R(1,4)	1.0889	1.0898	1.0908	1.0907	1.0861	1.0888	1.0889	1.0888	1.0879	1.0879	1.0864	1.0863	1.0863
R(1,5)	1.9705	1.9358	1.9258	1.9279	1.9621	1.9412	1.9414	1.9415	1.9342	1.9339	1.9337	1.9337	1.9337
A(2,1,3)	109.2798	108.706	108.2568	108.3836	108.615	108.7311	108.7504	108.7568	108.7312	108.7064	108.7594	108.7695	108.7734
A(2,1,4)	109.2876	111.4487	111.0294	111.2751	108.6064	111.3907	108.7472	108.7537	108.7255	108.7397	108.7565	108.767	108.771
A(2,1,5)	106.3259	110.6331	111.0052	110.8673	107.1781	110.8012	106.309	106.3072	106.3058	106.3091	106.2407	106.2352	106.2335
A(3,1,4)	111.6705	108.8803	108.4403	108.6089	111.039	108.7048	111.3917	111.3952	111.3374	111.3429	111.4044	111.428	111.4305
A(3,1,5)	110.0592	106.1787	106.7527	106.4241	110.6436	106.2641	110.7353	110.7282	110.7856	110.7645	110.7516	110.7319	110.7276
A(4,1,5)	110.0676	110.8161	111.1832	111.0976	110.6354	110.7722	110.7358	110.7288	110.784	110.8064	110.753	110.7337	110.7295
D(2,1,4,3)	-121.0292	-119.9027	-118.8153	-119.2238	-119.3644	-119.7845	-119.8364	-119.8506	-119.7651	-119.747	-119.8613	-119.8952	-119.9041
D(2,1,5,3)	118.244	117.7793	117.777	117.6614	118.2617	117.9479	117.9621	117.9648	117.964	117.9251	117.9416	117.94	117.9414
D(2,1,5,4)	-118.2577	-124.1367	-124.1283	-124.284	-118.2469	-124.1511	-117.9586	-117.9615	-117.9563	-117.9872	-117.939	-117.938	-117.9395
D(3,1,5,4)	123.4983	118.084	118.0947	118.0547	123.4914	117.901	124.0793	124.0737	124.0797	124.0877	124.1194	124.122	124.1191
Energy	-2439.97046371	-2440.19881305	-2440.21913977	-2440.21976933	-2442.35326252	-2442.38706049	-2442.38751643	-2442.38758615	-2442.38856593	-2442.38905106	-2442.39397838	-2442.39429307	-2442.39432258
ZPE Correction	0.035696	0.035429	0.034876	0.035555	0.03534	0.035119	0.035096	0.035057	0.035037	0.035037	0.035068	0.035057	0.03506

S10c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0895	1.0906	1.0915	1.0914	1.0866	1.0893	1.0943	1.0894	1.0884	1.0934	1.092	1.0917	1.092
R(1,3)	1.0947	1.095	1.0963	1.0963	1.087	1.0895	1.0896	1.0896	1.0889	1.0887	1.0872	1.0869	1.0872
R(1,4)	1.0896	1.0905	1.0916	1.0912	1.0921	1.0941	1.0896	1.0943	1.0933	1.0887	1.0873	1.0869	1.0872
R(1,5)	1.9742	1.9393	1.9288	1.9308	1.9658	1.9446	1.945	1.9447	1.9378	1.9376	1.9372	1.9372	1.9373
A(2,1,3)	109.3638	108.7655	108.3542	108.4006	111.0535	111.3538	108.7843	111.3637	111.3142	108.761	108.7901	108.7397	108.8064
A(2,1,4)	111.6912	111.4264	110.9735	111.2212	108.7673	108.8235	108.7815	108.8623	108.9801	108.7575	108.7876	108.7849	108.8043
A(2,1,5)	110.0298	110.6282	111.078	110.9492	110.7309	110.8003	106.3313	110.8522	110.983	106.3334	106.2689	106.3143	106.2605
A(3,1,4)	109.3231	108.8812	108.3649	108.537	108.5222	108.6994	111.372	108.6495	108.5523	111.3242	111.3808	111.4081	111.4103
A(3,1,5)	106.3042	106.2175	106.8296	106.4951	110.4825	110.6813	110.7022	110.6361	110.4909	110.7488	110.7209	110.772	110.6935
A(4,1,5)	109.9783	110.7498	111.0745	111.0571	107.1622	106.3137	110.703	106.3067	106.3542	110.7493	110.7224	110.6516	110.6955
D(2,1,4,3)	-121.1721	-119.9633	-118.8546	-119.1667	-120.9292	-121.4342	-119.8884	-121.4394	-121.3912	-119.8145	-119.9049	-119.8575	-119.9541
D(2,1,5,3)	118.3159	117.87	117.9795	117.767	123.4638	124.0379	117.998	124.0554	123.9809	117.9961	117.9784	117.9719	117.9784
D(2,1,5,4)	-123.4439	-124.0574	-124.03	-124.2443	-118.4842	-118.0869	-117.995	-118.1569	-118.3965	-117.9922	-117.9762	-117.9618	-117.977
D(3,1,5,4)	118.2402	118.0725	117.9905	117.9887	118.052	117.8753	124.007	117.7876	117.6226	124.0116	124.0454	124.0663	124.0446
Energy	-2438.99400732	-2439.22247002	-2439.24290233	-2439.24353523	-2441.37386625	-2441.40773514	-2441.40826863	-2441.40834232	-2441.40917442	-2441.40974443	-2441.41459652	-2441.41496823	-2441.4149985
ZPE Correction	0.035627	0.035372	0.035372	0.035501	0.035287	0.035053	0.035055	0.035062	0.034952	0.034974	0.035007	0.03499	0.034983

S10d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0966	1.0971	1.1033	1.0981	1.0934	1.0958	1.0959	1.0959	1.0949	1.1	1.0937	1.0985	1.0985
R(1,3)	1.1018	1.1017	1.0984	1.1033	1.0991	1.1007	1.1009	1.1009	1.0947	1.0951	1.0985	1.0936	1.0936
R(1,4)	1.0967	1.0971	1.0984	1.0986	1.0938	1.0958	1.0959	1.0959	1.0997	1.0951	1.0936	1.0936	1.0936
R(1,5)	2.0102	1.9683	1.9574	1.9604	1.999	1.9736	1.9737	1.9738	1.966	1.9663	1.9653	1.9651	1.9652
A(2,1,3)	109.6732	108.9528	108.5084	108.8766	109.0389	108.8545	108.869	108.8814	111.4754	108.8596	108.8155	108.8898	108.8933
A(2,1,4)	111.9965	111.576	108.4995	111.4587	111.3327	111.5249	111.5415	111.5445	108.7413	108.8589	111.5248	108.8901	108.8937
A(2,1,5)	109.7291	110.6272	106.6045	111.0269	110.5172	110.5802	110.5943	110.5954	110.5598	106.228	110.5582	106.145	106.1406
A(3,1,4)	109.6341	108.922	111.1977	108.459	108.7584	108.9079	108.8868	108.8861	108.9406	111.4957	108.9262	111.5612	111.5643
A(3,1,5)	105.8967	105.9857	110.9342	106.2717	106.8559	106.1593	106.1608	106.1588	110.7756	110.6139	106.1738	110.5886	110.5857
A(4,1,5)	109.7277	110.5933	110.9271	110.5637	110.2097	110.6391	110.6127	110.599	106.1725	110.6136	110.6674	110.5895	110.5866
D(2,1,4,3)	-121.9792	-120.3163	-119.2614	-119.8475	-120.1645	-120.1527	-120.1673	-120.1842	-121.6792	-120.1088	-120.1161	-120.2077	-120.2162
D(2,1,5,3)	118.2946	117.9584	117.9528	118.2472	118.5108	117.9171	117.9426	117.9569	124.09	117.9807	117.8674	117.9553	117.9553
D(2,1,5,4)	-123.4577	-124.1375	-117.9382	-124.2504	-123.4813	-124.0712	-124.0838	-124.0787	-117.7792	-117.9798	-124.0755	-117.9561	-117.9563
D(3,1,5,4)	118.2478	117.9041	124.1091	117.5024	118.0079	118.0118	117.9735	117.9644	118.1308	124.0395	118.057	124.0886	124.0884
Energy	-2440.20834163	-2440.43047602	-2440.45170788	-2440.45239959	-2442.57306575	-2442.60595409	-2442.60670463	-2442.60675414	-2442.60795169	-2442.60873845	-2442.61255927	-2442.61307406	-2442.61310045
ZPE Correction	0.033578	0.0336	0.033679	0.033799	0.034314	0.033525	0.033594	0.033533	0.033482	0.03365	0.033188	0.033279	0.03329

S10e – B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0912	1.092	1.0932	1.0983	1.0936	1.0906	1.0912	1.0907	1.0897	1.0898	1.088	1.0935	1.0887
R(1,3)	1.0964	1.0967	1.0982	1.093	1.0882	1.0957	1.0958	1.0958	1.0948	1.0949	1.0932	1.0883	1.0934
R(1,4)	1.0909	1.0919	1.0929	1.093	1.0882	1.0905	1.0904	1.0905	1.0896	1.0896	1.0881	1.0883	1.0879
R(1,5)	1.9847	1.9496	1.9394	1.942	1.9745	1.9546	1.955	1.9546	1.9478	1.9477	1.947	1.9475	1.9478
A(2,1,3)	109.403	108.9207	108.3916	108.658	108.7635	108.8187	108.6171	108.7938	108.7961	108.7943	108.9159	108.9039	108.6459
A(2,1,4)	111.8228	111.5097	111.1224	108.6533	108.7574	111.4606	111.4734	111.477	111.4124	111.4236	111.4191	108.9036	111.5027
A(2,1,5)	109.7785	110.5472	110.8452	106.3157	107.0729	110.5969	110.2976	110.5761	110.6576	110.6539	110.7541	106.144	110.2877
A(3,1,4)	109.5753	108.9423	108.5865	111.3809	111.1376	108.9164	109.1549	108.9358	108.8891	108.8878	108.8012	111.5087	109.1845
A(3,1,5)	106.1403	106.1393	106.6679	110.8277	110.4987	106.207	106.2514	106.19	106.1896	106.1885	106.1822	110.6018	106.1724
A(4,1,5)	109.9582	110.6095	111.0617	110.8268	110.4911	110.6705	110.8769	110.6954	110.724	110.7203	110.5967	110.6051	110.8742
D(2,1,4,3)	-121.48	-120.2481	-119.1275	-119.6549	-119.7032	-120.0736	-119.9868	-120.0657	-119.9978	-120.0017	-120.0934	-120.2012	-120.0606
D(2,1,5,3)	118.1375	117.967	117.802	117.9048	118.2981	117.9109	117.5394	117.8604	117.906	117.9012	118.0957	117.9784	117.5236
D(2,1,5,4)	-123.4266	-124.0075	-124.0446	-117.8987	-118.2865	-124.0228	-123.9727	-124.0468	-124.0421	-124.0511	-124.0287	-117.9799	-124.0013
D(3,1,5,4)	118.4358	118.0255	118.1534	124.1965	123.4154	118.0664	118.4879	118.0928	118.0519	118.0478	117.8756	124.0417	118.4751
Energy	-2438.83894334	-2439.06615184	-2439.08700438	-2439.08766455	-2441.22316948	-2441.25676723	-2441.25735762	-2441.25740912	-2441.25812689	-2441.25875152	-2441.26343121	-2441.26386683	-2441.26389947
ZPE Correction	0.035339	0.035098	0.035094	0.035023	0.034705	0.034702	0.034577	0.034748	0.034675	0.034664	0.034676	0.034653	0.034658

S10f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0954	1.0913	1.0924	1.0923	1.091	1.0951	1.0954	1.0954	1.0894	1.0948	1.0936	1.0937	1.0887
R(1,3)	1.0909	1.0958	1.0975	1.0975	1.0906	1.0903	1.0905	1.0905	1.0944	1.0898	1.0887	1.0888	1.0936
R(1,4)	1.0901	1.0913	1.093	1.0929	1.0867	1.0903	1.0905	1.0905	1.0899	1.0898	1.0888	1.0888	1.0888
R(1,5)	1.9774	1.9353	1.926	1.9281	1.9681	1.9441	1.9443	1.9444	1.9375	1.9374	1.9357	1.9363	1.9367
A(2,1,3)	109.0384	108.5622	108.3413	108.4574	107.7892	108.5846	108.5847	108.5846	108.7426	108.564	108.561	108.5785	108.6249
A(2,1,4)	109.5637	111.2912	110.9328	111.1968	110.1228	108.5778	108.578	108.5778	111.3175	108.5566	108.4905	108.5713	111.3764
A(2,1,5)	106.2583	111.0677	111.5981	111.4859	108.3506	106.3537	106.3347	106.326	111.1529	106.3584	106.3181	106.3062	110.9783
A(3,1,4)	111.656	108.4695	107.8461	108.0056	110.3073	111.3525	111.3857	111.3913	108.3561	111.3454	111.2905	111.3586	108.5276
A(3,1,5)	109.7762	106.2218	106.8596	106.5033	108.6789	110.8966	110.8881	110.8895	106.3871	110.9176	111.0329	110.9212	106.3035
A(4,1,5)	110.393	111.0329	111.0658	110.9838	111.4904	110.8937	110.8853	110.8867	110.7012	110.9152	110.9598	110.9191	110.8436
D(2,1,4,3)	-120.9026	-119.3649	-118.4959	-118.8887	-118.8508	-119.4985	-119.519	-119.5222	-119.5307	-119.4553	-119.3763	-119.4906	-119.5307
D(2,1,5,3)	117.7713	118.629	118.2691	118.1307	116.8669	117.876	117.8605	117.856	118.223	117.8654	117.8996	117.854	117.9384
D(2,1,5,4)	-118.7209	-124.4036	-124.3509	-124.5515	-121.3418	-117.8663	-117.851	-117.8464	-124.2581	-117.8553	-117.7762	-117.8443	-124.3113
D(3,1,5,4)	123.5078	117.7335	117.38	117.3177	121.7913	124.2577	124.2885	124.2976	117.5189	124.2792	124.3241	124.3017	117.7503
Energy	-2440.32342333	-2440.54684137	-2440.56884571	-2440.56953479	-2442.68732851	-2442.72153438	-2442.7225834	-2442.72260937	-2442.72315048	-2442.72422867	-2442.72794403	-2442.72867117	-2442.72871197
ZPE Correction	0.035475	0.034977	0.034357	0.034192	0.034781	0.034601	0.034553	0.034522	0.03408	0.034376	0.034414	0.034115	0.033738

S10g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0947	1.0905	1.0917	1.0917	1.0867	1.0941	1.0897	1.0944	1.0888	1.0889	1.0926	1.0926	1.0926
R(1,3)	1.0898	1.0948	1.0964	1.0965	1.0918	1.0896	1.0944	1.0898	1.0934	1.0937	1.088	1.0879	1.088
R(1,4)	1.0898	1.0906	1.0917	1.0916	1.0869	1.0896	1.0898	1.0898	1.089	1.0892	1.088	1.0879	1.088
R(1,5)	1.9779	1.94	1.9302	1.9323	1.9698	1.9474	1.948	1.9476	1.9409	1.941	1.9396	1.9399	1.9399
A(2,1,3)	109.3262	108.7482	108.2838	108.3616	108.7431	108.7529	108.7794	108.7525	108.8171	108.8269	108.7241	108.7497	108.7515
A(2,1,4)	109.3346	111.2864	110.9121	111.1744	111.0222	108.7492	111.3301	108.7488	111.2805	111.3037	108.7198	108.7461	108.748
A(2,1,5)	106.3122	110.8699	111.1816	111.0206	110.6549	106.4015	110.7642	106.3785	110.8854	110.867	106.3637	106.3423	106.3361
A(3,1,4)	111.6615	108.6705	108.2536	108.4522	108.6158	111.3019	108.7248	111.3261	108.6354	108.6435	111.2865	111.3335	111.3363
A(3,1,5)	110.0248	106.3371	106.9019	106.5227	107.1766	110.7367	106.3904	110.7353	106.3981	106.3942	110.7901	110.7508	110.7503
A(4,1,5)	110.0324	110.7592	111.1371	111.125	110.5105	110.7361	110.6878	110.7349	110.6598	110.6409	110.7898	110.7511	110.7508
D(2,1,4,3)	-121.1133	-119.7196	-118.6637	-119.0373	-119.5178	-119.7855	-119.8199	-119.7996	-119.7786	-119.8101	-119.7215	-119.7989	-119.8042
D(2,1,5,3)	118.2732	118.0477	117.9948	117.7749	118.4214	118.0198	118.0599	118.0051	118.1745	118.1741	117.9919	117.9888	117.9873
D(2,1,5,4)	-118.2871	-124.0566	-124.0713	-124.2851	-123.3904	-118.0151	-123.9865	-118.0006	-123.989	-123.9921	-117.9865	-117.9848	-117.9833
D(3,1,5,4)	123.4398	117.8957	117.9339	117.94	118.1883	123.965	117.9537	123.9943	117.8365	117.8338	124.0216	124.0264	124.0294
Energy	-2439.49280071	-2439.71814264	-2439.73999045	-2439.74064778	-2441.86942441	-2441.90361329	-2441.90468376	-2441.90471412	-2441.90486919	-2441.90598503	-2441.90996026	-2441.9107334	-2441.91076432
ZPE Correction	0.03531	0.035095	0.035467	0.035023	0.034898	0.034778	0.034603	0.034764	0.034667	0.034394	0.034668	0.034658	0.034655

S10h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1034	1.0987	1.1051	1.0998	1.1005	1.1022	1.0967	1.0967	1.1013	1.1016	1.0948	1.1002	1.1002
R(1,3)	1.0978	1.1034	1.0997	1.105	1.0948	1.0971	1.097	1.1024	1.0961	1.0963	1.1002	1.0948	1.0949
R(1,4)	1.0976	1.0982	1.0997	1.0994	1.0948	1.0971	1.1024	1.097	1.096	1.0963	1.0946	1.095	1.0949
R(1,5)	1.9857	1.9491	1.9389	1.9415	1.9779	1.9555	1.9548	1.9549	1.9479	1.9482	1.9467	1.9476	1.9476
A(2,1,3)	109.1855	108.4653	108.2069	108.2212	108.553	108.643	111.5827	108.7002	108.6029	108.6328	108.5429	108.7466	108.6736
A(2,1,4)	109.3266	111.6199	108.1917	111.4719	108.5403	108.638	108.7005	111.5858	108.6523	108.6278	111.6176	108.586	108.6699
A(2,1,5)	106.0673	110.6098	106.6045	110.9612	106.9846	106.1354	111.0048	110.9961	106.1397	106.1181	110.8749	106.0446	106.0372
A(3,1,4)	111.8759	108.879	111.2089	108.4896	111.2519	111.5919	108.4669	108.4781	111.5056	111.5863	108.6507	111.6659	111.6669
A(3,1,5)	110.0341	106.0026	111.2176	106.2492	110.6904	110.8175	110.8001	106.0741	110.9051	110.8376	105.9907	110.8781	110.7933
A(4,1,5)	110.176	111.0572	111.208	111.2312	110.6768	110.8166	106.078	110.7991	110.8387	110.8379	110.9505	110.7147	110.7949
D(2,1,4,3)	-121.0704	-119.7093	-118.7053	-119.0666	-119.3748	-119.7559	-121.498	-119.7192	-119.6625	-119.7331	-119.6559	-119.8959	-119.8608
D(2,1,5,3)	117.9718	117.3796	117.7441	117.415	118.0984	117.7763	124.5658	117.903	117.7771	117.7646	117.603	117.8788	117.7429
D(2,1,5,4)	-118.2132	-124.5134	-117.7206	-124.7055	-118.0756	-117.7698	-117.9103	-124.5626	-117.801	-117.7587	-124.626	-117.6017	-117.7394
D(3,1,5,4)	123.815	118.107	124.5354	117.8795	123.826	124.454	117.524	117.5344	124.4219	124.4767	117.7711	124.5195	124.5177
Energy	-2438.57535222	-2438.80518122	-2438.82681707	-2438.82750056	-2440.95013539	-2440.9846197	-2440.9854419	-2440.98548985	-2440.98613432	-2440.9869925	-2440.99117054	-2440.99177808	-2440.99180507
ZPE Correction	0.034522	0.034252	0.034179	0.034204	0.034078	0.03389	0.033904	0.033937	0.033857	0.03383	0.033926	0.033845	0.033841

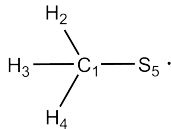
S10i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0974	1.0975	1.0935	1.0989	1.0943	1.0962	1.0909	1.0964	1.0953	1.0954	1.0938	1.0938	1.0938
R(1,3)	1.0919	1.0926	1.0988	1.0933	1.0887	1.0911	1.0962	1.0912	1.09	1.09	1.0885	1.0885	1.0885
R(1,4)	1.0919	1.0926	1.0935	1.0936	1.0887	1.0911	1.0912	1.0912	1.09	1.0901	1.0885	1.0885	1.0885
R(1,5)	1.981	1.9456	1.9353	1.9374	1.9711	1.9505	1.9501	1.9505	1.9437	1.9435	1.9431	1.9431	1.9432
A(2,1,3)	109.3836	108.8748	108.3721	108.6716	108.7033	108.8228	108.91	108.8183	108.7845	108.7964	108.8269	108.8413	108.8453
A(2,1,4)	109.3947	108.8748	111.1539	108.4414	108.6967	108.8212	111.482	108.8166	108.808	108.7799	108.8253	108.8401	108.8442
A(2,1,5)	106.1135	106.0208	111.0614	106.334	107.0101	106.1706	110.7826	106.1647	106.169	106.1566	106.103	106.091	106.0878
A(3,1,4)	111.8292	111.5586	108.3946	111.3555	111.1918	111.5168	108.7045	111.5259	111.4323	111.4454	111.5213	111.5515	111.5547
A(3,1,5)	109.9718	110.6614	106.6017	111.0511	110.5588	110.6646	106.2232	110.667	110.7363	110.7675	110.6897	110.6654	110.6614
A(4,1,5)	109.9817	110.6651	111.0759	110.801	110.5515	110.6665	110.5632	110.6689	110.7332	110.7157	110.6921	110.6683	110.6643
D(2,1,4,3)	-121.336	-120.1773	-119.0019	-119.5206	-119.6233	-120.0516	-120.0622	-120.0487	-119.943	-119.9476	-120.0622	-120.1085	-120.1181
D(2,1,5,3)	118.2003	117.9038	117.8563	118.0514	118.2217	117.9304	118.1278	117.9228	117.9216	117.9451	117.9092	117.9067	117.9074
D(2,1,5,4)	-118.2187	-117.9057	-124.2525	-117.6425	-118.2098	-117.9295	-124.1058	-117.9219	-117.9481	-117.8981	-117.9086	-117.9068	-117.9076
D(3,1,5,4)	123.5811	124.1905	117.8912	124.3061	123.5685	124.1401	117.7664	124.1553	124.1302	124.1568	124.1821	124.1865	124.185
Energy	-2439.17028147	-2439.39749227	-2439.41816256	-2439.41881261	-2441.54620824	-2441.57931722	-2441.57987764	-2441.57994147	-2441.58101443	-2441.58160776	-2441.58624573	-2441.58663548	-2441.58666186
ZPE Correction	0.03524	0.034988	0.035106	0.035072	0.034767	0.034668	0.034683	0.034669	0.034659	0.034603	0.034646	0.034635	0.034712

S10j – QCISD/cc-pVTZ

	QCISD/cc-pVTZ
R(1,2)	1.0854
R(1,3)	1.0896
R(1,4)	1.0851
R(1,5)	1.9421
A(2,1,3)	108.8779
A(2,1,4)	111.1628
A(2,1,5)	110.4269
A(3,1,4)	109.1139
A(3,1,5)	106.3920
A(4,1,5)	110.7262
D(2,1,4,3)	-120.0896
D(2,1,5,3)	117.9984
D(2,1,5,4)	-123.5610
D(3,1,5,4)	118.4406
Energy	-2439.90222600
ZPE Correction	0.035594

S11 – MeS.



S11a – B3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0967	1.0979	1.0985	1.0985	1.0919	1.0965	1.0966	1.0966	1.0956	1.0956	1.0941	1.0941	1.0941
R(1,3)	1.0908	1.0925	1.0929	1.0929	1.0855	1.0906	1.0908	1.0908	1.0896	1.0898	1.0881	1.0881	1.0881
R(1,4)	1.0908	1.0925	1.093	1.093	1.0855	1.0906	1.0909	1.0908	1.0896	1.0898	1.0881	1.0882	1.0882
R(1,5)	1.8774	1.8119	1.8123	1.8122	1.8786	1.8097	1.8094	1.8094	1.8021	1.8018	1.7977	1.7982	1.7983
A(2,1,3)	108.9289	107.9178	107.8793	107.8786	108.8571	107.9321	107.9233	107.939	107.9962	107.9911	107.9288	107.9453	107.9461
A(2,1,4)	108.9253	107.8976	107.8575	107.857	108.8583	107.9122	107.9035	107.9195	107.9789	107.9737	107.9103	107.9272	107.928
A(2,1,5)	106.6207	106.6899	106.7355	106.7158	106.4634	106.5189	106.5582	106.5543	106.4027	106.4329	106.4174	106.4192	106.4235
A(3,1,4)	111.3668	110.8005	110.8035	110.8087	111.6153	111.0252	110.9679	110.9759	111.0245	110.984	111.0213	111.0146	111.0163
A(3,1,5)	110.4347	111.6634	111.6777	111.6848	110.4452	111.6148	111.634	111.6168	111.607	111.6184	111.6649	111.6518	111.6483
A(4,1,5)	110.4251	111.6405	111.6534	111.6605	110.4405	111.5935	111.6123	111.5955	111.5885	111.5997	111.6462	111.6334	111.6298
D(2,1,4,3)	-120.1578	-117.938	-117.8691	-117.8709	-120.1799	-118.0922	-118.0435	-118.0768	-118.2103	-118.1776	-118.0847	-118.1113	-118.1137
D(2,1,5,3)	118.1962	117.6897	117.6788	117.6699	118.0246	117.5773	117.6008	117.6081	117.5804	117.5985	117.5393	117.5533	117.5549
D(2,1,5,4)	-118.1868	-117.6528	-117.6392	-117.6305	-118.0236	-117.5419	-117.5651	-117.573	-117.5496	-117.5676	-117.507	-117.5215	-117.523
D(3,1,5,4)	123.617	124.6575	124.682	124.6996	123.9518	124.8808	124.8341	124.8189	124.8701	124.8339	124.9537	124.9252	124.9221
Energy	-438.033746903	-438.064017623	-438.066716004	-438.066760496	-438.071434446	-438.099413986	-438.100324833	-438.100487994	-438.105036251	-438.105902437	-438.108039929	-438.108401311	-438.108472913
ZPE Correction	0.035904	0.035652	0.03552	0.035517	0.035598	0.035391	0.035362	0.035369	0.035352	0.035339	0.035377	0.035361	0.035356

S11b – B3P86

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0968	1.0976	1.098	1.098	1.0923	1.0966	1.0967	1.0967	1.0959	1.0959	1.0946	1.0946	1.0946
R(1,3)	1.0906	1.0922	1.0925	1.0925	1.0858	1.0907	1.0909	1.0906	1.0899	1.09	1.0885	1.0885	1.0885
R(1,4)	1.0906	1.0922	1.0925	1.0925	1.0858	1.0908	1.091	1.0913	1.0899	1.09	1.0885	1.0885	1.0886
R(1,5)	1.8597	1.7972	1.7973	1.7972	1.8597	1.7945	1.7944	1.7945	1.7872	1.787	1.7829	1.7836	1.7837
A(2,1,3)	108.6164	107.7184	107.6792	107.6842	108.5575	107.7227	107.7198	107.9924	107.8175	107.8152	107.7339	107.7588	107.7597
A(2,1,4)	108.6058	107.6942	107.6536	107.6589	108.5503	107.6985	107.6957	107.4674	107.7964	107.7942	107.7112	107.7366	107.7375
A(2,1,5)	106.7448	106.6917	106.729	106.7087	106.5967	106.4654	106.5012	106.5202	106.2925	106.3211	106.3008	106.2995	106.3055
A(3,1,4)	111.276	110.7933	110.7844	110.7904	111.4743	111.024	110.9709	110.9763	111.0549	111.0173	111.0611	111.0565	111.058
A(3,1,5)	110.7351	111.8525	111.8769	111.8784	110.7505	111.8359	111.8489	112.0485	111.8096	111.8176	111.8804	111.8601	111.8558
A(4,1,5)	110.7097	111.8283	111.8515	111.8533	110.7393	111.8132	111.826	111.5609	111.7903	111.7982	111.8607	111.8407	111.8363
D(2,1,4,3)	-119.5093	-117.5713	-117.495	-117.5075	-119.5215	-117.7084	-117.6734	-117.8687	-117.8997	-117.8743	-117.7504	-117.7933	-117.7959
D(2,1,5,3)	118.0573	117.5535	117.5422	117.5368	117.9079	117.4124	117.4376	117.8875	117.408	117.4268	117.3504	117.3687	117.3711
D(2,1,5,4)	-118.0308	-117.511	-117.4974	-117.4924	-117.8934	-117.3709	-117.3962	-116.9903	-117.3723	-117.3911	-117.3125	-117.3316	-117.3339
D(3,1,5,4)	123.9119	124.9355	124.9604	124.9708	124.1988	125.2167	125.1662	125.1222	125.2197	125.1821	125.3371	125.2997	125.295
Energy	-438.497532835	-438.527779699	-438.529469909	-438.5295136	-438.532300673	-438.560817039	-438.561918237	-438.562126984	-438.566746643	-438.567795428	-438.569674358	-438.570122102	-438.570211213
ZPE Correction	0.036174	0.035795	0.035696	0.035694	0.03581	0.035533	0.035516	0.035513	0.035482	0.035469	0.0355	0.035505	0.035486

S11c – B3PW91

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0974	1.0981	1.0985	1.0985	1.0926	1.0972	1.0973	1.0973	1.0964	1.0965	1.0953	1.0952	1.0953
R(1,3)	1.0913	1.0928	1.0931	1.0931	1.0864	1.0914	1.0917	1.0916	1.0906	1.0908	1.0893	1.0894	1.0894
R(1,4)	1.0913	1.0929	1.0932	1.0932	1.0864	1.0914	1.0917	1.0917	1.0906	1.0908	1.0893	1.0894	1.0894
R(1,5)	1.8625	1.7998	1.7998	1.7997	1.8628	1.7973	1.7971	1.7972	1.7902	1.7899	1.786	1.7866	1.7867
A(2,1,3)	108.6523	107.7494	107.7098	107.7167	108.6599	107.7718	107.7634	107.7828	107.8653	107.8611	107.7855	107.8052	107.806
A(2,1,4)	108.6424	107.7255	107.6844	107.6916	108.5704	107.7486	107.7401	107.7598	107.8453	107.841	107.7638	107.7839	107.7846
A(2,1,5)	106.746	106.7276	106.7698	106.7498	106.5782	106.475	106.5194	106.5171	106.3015	106.3356	106.3099	106.3142	106.3201
A(3,1,4)	111.2768	110.7698	110.7576	110.7633	111.468	111.012	110.9532	110.964	111.0437	111.0033	111.05	111.0423	111.0438
A(3,1,5)	110.6997	111.8192	111.8435	111.8432	110.7051	111.7918	111.8089	111.7863	111.7664	111.7751	111.8338	111.8173	111.8132
A(4,1,5)	110.6739	111.7947	111.8178	111.8178	110.6914	111.7695	111.7863	111.7641	111.7476	111.7561	111.8144	111.7981	111.794
D(2,1,4,3)	-119.5773	-117.6143	-117.5353	-117.551	-119.6571	-117.7912	-117.7427	-117.7842	-117.981	-117.9504	-117.8385	-117.8701	-117.8723
D(2,1,5,3)	118.0817	117.5947	117.5858	117.5818	117.9952	117.4535	117.4795	117.4893	117.4478	117.468	117.393	117.4105	117.4128
D(2,1,5,4)	-118.0559	-117.5522	-117.541	-117.5375	-117.8808	-117.4135	-117.4391	-117.4495	-117.4136	-117.4336	-117.3565	-117.3746	-117.3768
D(3,1,5,4)	123.8624	124.8531	124.8732	124.8807	124.124	125.1331	125.0813	125.0612	125.1386	125.0984	125.2505	125.2149	125.2105
Energy	-437.967654508	-437.997720668	-437.999482681	-437.999531438	-438.002262137	-438.030647661	-438.031703243	-438.031912437	-438.036647011	-438.037646536	-438.039424965	-438.039819916	-438.039910939
ZPE Correction	0.036184	0.035784	0.035685	0.035683	0.035816	0.035521	0.035496	0.035503	0.035461	0.035448	0.035476	0.03546	0.035454

S11d – B97D

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1045	1.105	1.1055	1.1056	1.1003	1.1038	1.1039	1.104	1.1029	1.103	1.1016	1.1016	1.1016
R(1,3)	1.0983	1.0998	1.1002	1.1002	1.0934	1.0977	1.0981	1.0979	1.0971	1.0974	1.0956	1.0959	1.0959
R(1,4)	1.0983	1.0998	1.1002	1.1003	1.0934	1.0979	1.0987	1.0981	1.0972	1.0974	1.0956	1.0959	1.0959
R(1,5)	1.8882	1.8167	1.8171	1.8171	1.8891	1.814	1.8139	1.8137	1.8069	1.8065	1.8014	1.8026	1.8027
A(2,1,3)	108.8452	107.732	107.6887	107.6898	108.7514	107.8038	107.9791	107.8318	107.8298	107.8263	107.6648	107.8094	107.7823
A(2,1,4)	108.8434	107.7037	107.6588	107.6602	108.7557	107.6711	107.4836	107.6689	107.8063	107.8024	107.7525	107.7344	107.7574
A(2,1,5)	106.4114	106.6249	106.6775	106.6529	106.2591	106.3613	106.5052	106.3958	106.3488	106.3738	106.3171	106.3632	106.3689
A(3,1,4)	111.5328	110.8406	110.845	110.8516	111.7666	111.1229	111.0145	111.0714	111.0794	111.0431	111.1034	111.0651	111.0648
A(3,1,5)	110.5286	111.8527	111.8672	111.874	110.5632	111.8605	112.0319	111.8652	111.7637	111.7742	111.7905	111.8374	111.8065
A(4,1,5)	110.5169	111.821	111.8345	111.8414	110.5581	111.7349	111.5501	111.7268	111.7391	111.749	111.9181	111.7514	111.7814
D(2,1,4,3)	-120.1039	-117.6198	-117.5433	-117.5491	-120.0754	-117.8458	-117.8839	-117.8493	-117.9346	-117.9074	-117.7156	-117.8583	-117.839
D(2,1,5,3)	118.0249	117.5294	117.517	117.5071	117.843	117.4605	117.8532	117.5177	117.4321	117.4487	117.2289	117.456	117.41
D(2,1,5,4)	-118.0165	-117.478	-117.463	-117.4535	-117.8454	-117.2332	-116.9951	-117.2469	-117.3906	-117.4063	-117.4029	-117.3194	-117.3665
D(3,1,5,4)	123.9586	124.9926	125.02	125.0393	124.3116	125.3063	125.1517	125.2354	125.1772	125.145	125.3681	125.2246	125.2235
Energy	-438.002230891	-438.030113832	-438.032702917	-438.032745269	-438.040694091	-438.066616396	-438.067439738	-438.067598764	-438.071947167	-438.072757356	-438.074751079	-438.075034486	-438.075103285
ZPE Correction	0.035074	0.034696	0.034572	0.034564	0.03469	0.03444	0.034304	0.034375	0.034311	0.034305	0.034382	0.034294	0.034326

S11e– B971

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0987	1.0998	1.1003	1.1003	1.0944	1.0986	1.0987	1.0987	1.0979	1.098	1.0965	1.0966	1.0966
R(1,3)	1.0926	1.0941	1.0945	1.0945	1.0876	1.0924	1.0927	1.0927	1.0917	1.0919	1.0901	1.0903	1.0903
R(1,4)	1.0926	1.0942	1.0945	1.0946	1.0876	1.0925	1.0927	1.0927	1.0917	1.0919	1.0902	1.0903	1.0903
R(1,5)	1.8763	1.8134	1.8136	1.8135	1.8761	1.8115	1.8112	1.8112	1.8027	1.8024	1.7986	1.7996	1.7997
A(2,1,3)	108.9195	107.9445	107.9011	107.9036	108.8253	107.9699	107.9591	107.9768	108.0292	108.0219	108.0042	107.988	107.9887
A(2,1,4)	108.9138	107.9239	107.8793	107.882	108.8244	107.9511	107.9398	107.9579	108.0129	108.0053	107.9005	107.971	107.9717
A(2,1,5)	106.5423	106.5725	106.6166	106.5957	106.3798	106.3613	106.3985	106.3919	106.2022	106.2319	106.2468	106.2139	106.2199
A(3,1,4)	111.4586	110.9299	110.9255	110.9311	111.6842	111.1677	111.1122	111.1207	111.1863	111.1476	111.1567	111.1813	111.1829
A(3,1,5)	110.4352	111.6278	111.6508	111.6552	110.4812	111.5792	111.6008	111.5827	111.5854	111.5986	111.6985	111.6212	111.617
A(4,1,5)	110.424	111.6052	111.6271	111.6317	110.475	111.5593	111.5802	111.5626	111.5686	111.5813	111.5719	111.6043	111.6
D(2,1,4,3)	-120.196	-118.0598	-117.9778	-117.9856	-120.1612	-118.2436	-118.1916	-118.2291	-118.3646	-118.3287	-118.2479	-118.2857	-118.2879
D(2,1,5,3)	118.1397	117.6315	117.6185	117.6112	117.9576	117.509	117.5299	117.5375	117.4884	117.5044	117.5456	117.4649	117.4672
D(2,1,5,4)	-118.1268	-117.5945	-117.5792	-117.5724	-117.9531	-117.4757	-117.4956	-117.504	-117.4599	-117.4753	-117.3533	-117.4356	-117.4377
D(3,1,5,4)	123.7335	124.774	124.8023	124.8164	124.0894	125.0153	124.9745	124.9586	125.0517	125.0203	125.1011	125.0994	125.0951
Energy	-437.961984336	-437.990808152	-437.992929571	-437.992969786	-437.996766504	-438.024102313	-438.025021332	-438.025194234	-438.029998141	-438.030867728	-438.032498536	-438.032833034	-438.032908441
ZPE Correction	0.035511	0.035491	0.035382	0.035381	0.03526	0.035226	0.035204	0.03521	0.035195	0.035185	0.035176	0.035202	0.035195

S11f – HCTH

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0983	1.0994	1.1	1.1	1.0872	1.0981	1.0923	1.0928	1.0979	1.0982	1.0968	1.091	1.0912
R(1,3)	1.0923	1.0942	1.0946	1.0946	1.0872	1.0925	1.098	1.0987	1.0919	1.0923	1.0912	1.0912	1.0971
R(1,4)	1.0924	1.0942	1.0946	1.0946	1.0936	1.0923	1.0922	1.0929	1.092	1.0923	1.091	1.0971	1.0913
R(1,5)	1.8585	1.7912	1.7916	1.7915	1.8578	1.7887	1.788	1.7882	1.7842	1.7838	1.7779	1.778	1.7778
A(2,1,3)	108.4679	107.3908	107.3334	107.3293	111.4561	107.4798	107.3823	107.383	107.5531	107.5418	107.4723	110.9142	107.4826
A(2,1,4)	108.4564	107.3566	107.2977	107.2936	108.4314	107.4166	110.9705	110.9193	107.5235	107.5114	107.3785	107.4749	110.8857
A(2,1,5)	106.7293	106.7392	106.7996	106.7758	110.8875	106.5341	112.1872	112.1186	106.3959	106.4203	106.443	112.2043	112.1626
A(3,1,4)	111.2483	110.707	110.7116	110.7175	108.4157	110.9731	107.397	107.39	111.0179	110.9811	110.9193	107.3597	107.3928
A(3,1,5)	110.8947	112.1811	112.2041	112.216	110.8749	112.0838	106.5795	106.5881	112.0298	112.0483	112.1874	112.105	106.5258
A(4,1,5)	110.8772	112.1491	112.1712	112.1829	106.5907	112.0327	111.9966	112.1145	112.0043	112.0218	112.1078	106.4492	112.0682
D(2,1,4,3)	-119.2148	-116.9311	-116.8305	-116.8264	-121.1541	-117.2186	-117.0883	-117.0569	-117.3953	-117.354	-117.1575	-119.3745	-117.16
D(2,1,5,3)	117.9567	117.3664	117.3466	117.3336	124.3714	117.2953	117.2615	117.2302	117.2706	117.2817	117.2869	125.5868	117.3365
D(2,1,5,4)	-117.9332	-117.3074	-117.2853	-117.272	-117.8271	-117.1912	-125.5629	-125.5334	-117.221	-117.2307	-117.1306	-117.3031	-125.4867
D(3,1,5,4)	124.1101	125.3262	125.368	125.3944	117.8015	125.5135	117.1756	117.2364	125.5085	125.4876	125.5825	117.1101	117.1768
Energy	-438.074585163	-438.103981195	-438.107084516	-438.107135639	-438.111384228	-438.139234325	-438.139998643	-438.140112734	-438.144680894	-438.14539245	-438.147081164	-438.147314229	-438.14736925
ZPE Correction	0.035741	0.03537	0.035226	0.035218	0.035335	0.035063	0.034943	0.0349	0.034899	0.034913	0.034901	0.034956	0.034725

S11g – O3LYP

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0972	1.0983	1.0989	1.0989	1.0929	1.0973	1.0976	1.0976	1.0969	1.0972	1.096	1.09	1.0901
R(1,3)	1.0913	1.0931	1.0935	1.0935	1.0864	1.0915	1.0919	1.0918	1.091	1.0914	1.09	1.096	1.096
R(1,4)	1.0913	1.0931	1.0935	1.0936	1.0864	1.0915	1.092	1.0919	1.091	1.0914	1.0901	1.0902	1.0902
R(1,5)	1.8654	1.7996	1.7998	1.7997	1.8647	1.7978	1.7975	1.7969	1.7912	1.7908	1.786	1.7862	1.7863
A(2,1,3)	108.6788	107.6434	107.5906	107.5943	108.6268	107.7418	107.7111	107.7362	107.7918	107.781	107.7188	107.7296	107.7333
A(2,1,4)	108.6687	107.6169	107.5623	107.5662	108.6219	107.7161	107.6863	107.6331	107.7696	107.7586	107.6271	110.9803	110.9808
A(2,1,5)	106.7362	106.7461	106.8145	106.7925	106.528	106.4673	106.5166	106.5638	106.3172	106.354	106.379	111.9642	111.9603
A(3,1,4)	111.2794	110.7509	110.7371	110.7414	111.535	111.0439	110.9765	110.9577	111.0655	111.0223	110.9954	107.6279	107.6272
A(3,1,5)	110.6726	111.9199	111.9452	111.9497	110.6835	111.8092	111.848	111.8864	111.818	111.8331	111.9657	106.3997	106.4087
A(4,1,5)	110.6568	111.8928	111.9164	111.9211	110.6735	111.7844	111.8237	111.7866	111.7968	111.8115	111.8606	111.8477	111.8401
D(2,1,4,3)	-119.6285	-117.4115	-117.3081	-117.3172	-119.6903	-117.7532	-117.6604	-117.6482	-117.8583	-117.8142	-117.6447	-117.6498	-117.6542
D(2,1,5,3)	118.0931	117.533	117.5249	117.5183	117.9146	117.4221	117.436	117.5157	117.3965	117.4138	117.4255	117.4503	117.4582
D(2,1,5,4)	-118.0724	-117.4861	-117.4747	-117.4685	-117.9034	-117.3777	-117.3928	-117.3371	-117.3584	-117.3752	-117.2584	-125.2848	-125.2765
D(3,1,5,4)	123.8345	124.981	125.0004	125.0132	124.182	125.2002	125.1712	125.1472	125.2452	125.211	125.3161	117.2649	117.2654
Energy	-437.996961977	-438.025953931	-438.028856928	-438.028902078	-438.031704881	-438.059633343	-438.060466505	-438.060610935	-438.065386592	-438.066157319	-438.067603524	-438.06782199	-438.067887532
ZPE Correction	0.036275	0.035798	0.035681	0.035671	0.035947	0.035538	0.035492	0.035487	0.035422	0.035395	0.03541	0.03536	0.035354

S11h – PBE

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.1063	1.107	1.1076	1.1076	1.1021	1.1057	1.1059	1.1059	1.1051	1.1052	1.104	1.104	1.104
R(1,3)	1.0996	1.1011	1.1016	1.1016	1.0946	1.0993	1.0996	1.0995	1.0986	1.0988	1.0974	1.0974	1.0975
R(1,4)	1.0996	1.1011	1.1016	1.1016	1.0946	1.0993	1.0996	1.0996	1.0986	1.0989	1.0974	1.0975	1.0975
R(1,5)	1.871	1.8064	1.8069	1.8067	1.8716	1.8042	1.8039	1.8041	1.7968	1.7965	1.7926	1.7929	1.793
A(2,1,3)	108.4947	107.466	107.4068	107.4052	108.3793	107.4855	107.4634	107.4962	107.5944	107.587	107.5229	107.5326	107.5342
A(2,1,4)	108.4765	107.429	107.367	107.3657	108.3648	107.4494	107.4269	107.4426	107.5637	107.5562	107.4917	107.5017	107.5032
A(2,1,5)	106.5331	106.5314	106.6053	106.576	106.365	106.3229	106.3614	106.353	106.1417	106.173	106.1276	106.1378	106.143
A(3,1,4)	111.4833	110.9706	110.9517	110.9597	111.731	111.2309	111.1647	111.1713	111.2729	111.2269	111.288	111.2758	111.2776
A(3,1,5)	110.8477	112.0797	112.1113	112.122	110.9042	112.0241	112.0606	112.0516	111.9813	111.9973	112.0455	112.038	112.0334
A(4,1,5)	110.8226	112.043	112.0726	112.0835	110.884	111.9908	112.0265	111.9923	111.9532	111.9688	112.0172	112.0098	112.0051
D(2,1,4,3)	-119.4022	-117.208	-117.0898	-117.0913	-119.3379	-117.3875	-117.3106	-117.3634	-117.6115	-117.5723	-117.4899	-117.5009	-117.5048
D(2,1,5,3)	117.8476	117.2748	117.2656	117.2515	117.6412	117.1417	117.158	117.1877	117.1406	117.1591	117.0803	117.0942	117.0968
D(2,1,5,4)	-117.8124	-117.2102	-117.1964	-117.1828	-117.6132	-117.0805	-117.0957	-117.0912	-117.0889	-117.1069	-117.0277	-117.0419	-117.0444
D(3,1,5,4)	124.34	125.515	125.538	125.5657	124.7456	125.7778	125.7463	125.7211	125.7705	125.734	125.892	125.8639	125.8588
Energy	-437.782137861	-437.810296125	-437.81322882	-437.813280819	-437.81986662	-437.845836921	-437.846702642	-437.846872624	-437.851589893	-437.85241484	-437.854252788	-437.85453843	-437.854611748
ZPE Correction	0.035058	0.034653	0.03453	0.034524	0.034764	0.034399	0.03436	0.034353	0.03433	0.034308	0.034343	0.034323	0.034319

S11i – τ HCTHhybrid

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
R(1,2)	1.0992	1.1004	1.1008	1.1008	1.095	1.099	1.0991	1.0991	1.0979	1.0983	1.0968	1.0968	1.0968
R(1,3)	1.093	1.0948	1.0951	1.0951	1.0882	1.0927	1.0931	1.0931	1.0914	1.0922	1.0905	1.0905	1.0906
R(1,4)	1.0933	1.0948	1.0951	1.0951	1.0882	1.0928	1.0931	1.0931	1.0927	1.0922	1.0905	1.0906	1.0906
R(1,5)	1.8733	1.8102	1.8104	1.8103	1.8718	1.8073	1.8074	1.8075	1.7983	1.7984	1.7952	1.7958	1.7959
A(2,1,3)	108.907	107.8711	107.8276	107.8316	108.722	107.8907	107.8817	107.9	108.4783	107.9455	107.8927	107.913	107.9139
A(2,1,4)	108.8031	107.8495	107.8048	107.8091	108.7197	107.8435	107.8609	107.8796	107.4952	107.9277	107.8746	107.8951	107.896
A(2,1,5)	106.551	106.5549	106.5974	106.5746	106.3683	106.3341	106.3809	106.3756	106.4925	106.2277	106.2056	106.2052	106.2122
A(3,1,4)	111.4092	110.9097	110.9045	110.9109	111.6722	111.1644	111.1109	111.1198	111.0215	111.1381	111.1849	111.179	111.1806
A(3,1,5)	110.5589	111.7149	111.739	111.7425	110.5936	111.6949	111.6822	111.6628	112.1044	111.6769	111.712	111.6962	111.6914
A(4,1,5)	110.4623	111.6915	111.7145	111.7182	110.5861	111.6448	111.6609	111.642	111.0039	111.6592	111.6948	111.6791	111.6742
D(2,1,4,3)	-120.0774	-117.9144	-117.832	-117.8429	-119.9566	-118.0795	-118.0487	-118.0874	-118.499	-118.1825	-118.1126	-118.1466	-118.1491
D(2,1,5,3)	118.1962	117.5798	117.5662	117.5591	117.8873	117.4596	117.47	117.4784	118.4907	117.452	117.394	117.4098	117.4125
D(2,1,5,4)	-118.0202	-117.541	-117.5254	-117.5187	-117.8807	-117.376	-117.4336	-117.4427	-116.7125	-117.4211	-117.3631	-117.3792	-117.3818
D(3,1,5,4)	123.7836	124.8792	124.9083	124.9222	124.232	125.1645	125.0964	125.0789	124.7969	125.1269	125.2429	125.211	125.2057
Energy	-437.979921739	-438.008823199	-438.010834483	-438.010878321	-438.016646143	-438.043460165	-438.044404597	-438.044593367	-438.04927288	-438.050183511	-438.052168064	-438.052511238	-438.05259165
ZPE Correction	0.034493	0.035131	0.035039	0.035041	0.03448	0.034918	0.034881	0.034886	0.034524	0.034881	0.034932	0.034913	0.034904

S11j – QCISD/cc-pVTZ

	QCISD/cc-pVTZ
R(1,2)	1.0921
R(1,3)	1.0868
R(1,4)	1.0872
R(1,5)	1.8047
A(2,1,3)	108.4533
A(2,1,4)	108.2515
A(2,1,5)	106.4827
A(3,1,4)	110.8511
A(3,1,5)	111.4136
A(4,1,5)	111.2019
D(2,1,4,3)	-118.8334
D(2,1,5,3)	118.0739
D(2,1,5,4)	-117.7167
D(3,1,5,4)	124.2094
Energy	-437.5123726
ZPE Correction	0.036066

S12 – HO·

S12a – O–H Bond Lengths

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	0.9969	0.9797	0.9798	0.98	0.9916	0.9752	0.9759	0.9759	0.975	0.976	0.9729	0.9742	0.9742
B3P86	0.9932	0.9764	0.9769	0.9771	0.989	0.9728	0.9735	0.9735	0.9726	0.9737	0.9712	0.9721	0.9721
B3PW91	0.9936	0.9767	0.977	0.9773	0.9892	0.973	0.9737	0.9737	0.9729	0.9739	0.9714	0.9723	0.9723
B97D	1.0033	0.9837	0.9838	0.9841	0.9976	0.9792	0.9798	0.9798	0.9789	0.9799	0.9772	0.9782	0.9783
B971	0.9945	0.9778	0.9779	0.9781	0.9894	0.9735	0.9742	0.9742	0.9733	0.9744	0.9717	0.9728	0.9728
HCTH	0.9975	0.9786	0.9786	0.9789	0.9914	0.9742	0.9748	0.9748	0.974	0.9751	0.9718	0.9735	0.9735
O3LYP	0.9952	0.9777	0.9775	0.9778	0.9896	0.9736	0.974	0.974	0.9734	0.9743	0.9712	0.9726	0.9727
PBE	1.007	0.988	0.9882	0.9885	1.0019	0.984	0.9846	0.9846	0.9838	0.9849	0.9817	0.9831	0.9832
tHCTHhybrid	0.9964	0.9787	0.9789	0.9792	0.9913	0.9743	0.975	0.975	0.9742	0.9752	0.9727	0.9735	0.9735
QCISD/cc-pVTZ	0.9692												

S12b – Electronic Energies

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	-75.708548871	-75.7284822968	-75.7390145636	-75.7391301043	-75.7361018694	-75.7545273608	-75.7623379915	-75.7624123365	-75.7564572036	-75.7640647217	-75.7611531098	-75.7662003967	-75.7662448525
B3P86	-75.8641176801	-75.8844144862	-75.8929014761	-75.8930173489	-75.8904884051	-75.9094486037	-75.9156085463	-75.9156987766	-75.9114702388	-75.9174570323	-75.915585233	-75.9195657064	-75.9196198212
B3PW91	-75.6790665781	-75.6994213879	-75.7081202335	-75.7082419338	-75.7052374602	-75.7242406543	-75.730622892	-75.7307209814	-75.7262894118	-75.7324901669	-75.7304083144	-75.7345832549	-75.7346424487
B97D	-75.664777112	-75.6838816111	-75.6941152907	-75.6942445819	-75.6921108772	-75.7098085068	-75.7175328552	-75.7176230236	-75.711752869	-75.7192831028	-75.7163004523	-75.721339802	-75.7213934029
B971	-75.6837682337	-75.7038704425	-75.7130733358	-75.7131849422	-75.7098321879	-75.7285924223	-75.7356183406	-75.7357035336	-75.7304771228	-75.7373115826	-75.7347871455	-75.7393518054	-75.7394033053
HCTH	-75.6878575923	-75.708098819	-75.7190026306	-75.7191098451	-75.7140211357	-75.7324285662	-75.7412275803	-75.741310144	-75.7344604126	-75.7430261724	-75.7393397315	-75.7450441887	-75.7450951269
O3LYP	-75.6818463681	-75.7020807296	-75.7128869669	-75.713010518	-75.7075610968	-75.7262640552	-75.735084561	-75.7351877481	-75.7282773192	-75.7368562592	-75.7329326071	-75.7388475905	-75.7389108229
PBE	-75.6223164193	-75.6418230174	-75.6534352138	-75.6535633489	-75.6494613234	-75.6673046659	-75.6761102286	-75.6761951287	-75.6693653257	-75.6779536481	-75.674323774	-75.6800576641	-75.6801105702
tHCTHhybrid	-75.6867152609	-75.7064818477	-75.7154066922	-75.7155308197	-75.7138691073	-75.7323534295	-75.738900721	-75.7389965927	-75.7342333193	-75.7405993797	-75.7384538655	-75.7427190919	-75.7427744894
QCISD/cc-pVTZ	-75.6328418												

S12c – Zero Point Vibrational Energy Corrections

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	0.0079	0.008421	0.008438	0.008433	0.00791	0.00844	0.00845	0.008451	0.008441	0.008443	0.00848	0.008461	0.008461
B3P86	0.008019	0.008539	0.008541	0.008538	0.008006	0.00854	0.008539	0.008541	0.00854	0.008533	0.008557	0.008544	0.008544
B3PW91	0.008004	0.008526	0.008531	0.008527	0.007991	0.008526	0.008528	0.008529	0.008526	0.008521	0.008543	0.008532	0.008533
B97D	0.007684	0.008236	0.008251	0.008245	0.007693	0.008258	0.008267	0.008268	0.008264	0.008266	0.008295	0.008281	0.008281
B971	0.007992	0.008518	0.00853	0.008526	0.008002	0.008528	0.008533	0.008534	0.008528	0.008526	0.008551	0.008535	0.008536
HCTH	0.007803	0.008372	0.008388	0.008381	0.007838	0.008391	0.0084	0.008401	0.008395	0.008395	0.00843	0.008406	0.008406
O3LYP	0.007916	0.008465	0.008485	0.008477	0.007942	0.008473	0.008489	0.008489	0.008475	0.008482	0.008508	0.008491	0.008491
PBEPBE	0.007655	0.008199	0.008213	0.008207	0.007654	0.008208	0.00822	0.008221	0.008212	0.008216	0.00825	0.008231	0.008232
tHCTHhyb	0.00791	0.00845	0.008458	0.008454	0.007907	0.008458	0.008462	0.008464	0.008457	0.008455	0.008484	0.008473	0.008473
QCISD/cc-pVTZ	0.008596												

S13 – HSe.

S13a – Se–H Bond Lengths

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	1.4871	1.4657	1.4665	1.47	1.4926	1.4766	1.4767	1.4768	1.4748	1.475	1.4739	1.4739	1.474
B3P86	1.4823	1.4612	1.4616	1.4641	1.4882	1.4717	1.4718	1.4719	1.47	1.47	1.47	1.47	1.47
B3PW91	1.4836	1.4625	1.4629	1.4655	1.4894	1.4736	1.4738	1.4739	1.472	1.4721	1.4715	1.4715	1.4716
B97D	1.4934	1.47	1.47	1.4738	1.4997	1.4814	1.4816	1.4817	1.4796	1.4798	1.4785	1.4786	1.4786
B971	1.4849	1.4634	1.4641	1.4674	1.4909	1.4757	1.4759	1.476	1.4743	1.4744	1.4737	1.4737	1.4738
HCTH	1.4861	1.4624	1.4633	1.4666	1.4953	1.476	1.4764	1.4765	1.4736	1.4739	1.4733	1.4735	1.4736
O3LYP	1.4823	1.4613	1.4618	1.4644	1.4916	1.474	1.4743	1.4745	1.472	1.4723	1.4719	1.472	1.4721
PBEPBE	1.4975	1.475	1.4759	1.4792	1.5048	1.4862	1.4865	1.4866	1.4842	1.4845	1.4847	1.484	1.484
tHCTHhybrid	1.4851	1.4626	1.4632	1.4665	1.4908	1.4742	1.4743	1.4744	1.4726	1.4728	1.4716	1.4716	1.4717
QCISD/cc-pvtz	1.4614												

S13b – Electronic Energies

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	-2399.71372197	-2399.93635615	-2399.95259664	-2399.95296861	-2402.09031222	-2402.1171766	-2402.11758295	-2402.11761481	-2402.11652355	-2402.11690997	-2402.12035909	-2402.12072189	-2402.1207423
B3P86	-2400.50813	-2400.73098212	-2400.74631956	-2400.74666866	-2402.8873223	-2402.9145078	-2402.91473678	-2402.9147671	-2402.91394029	-2402.91415387	-2402.91783849	-2402.91802317	-2402.91804333
B3PW91	-2399.69163324	-2399.91476214	-2399.93019901	-2399.93055273	-2402.06832754	-2402.09557195	-2402.09584338	-2402.09587716	-2402.09499187	-2402.09524875	-2402.09888275	-2402.09911543	-2402.09913647
B97D	-2400.92226136	-2401.13907928	-2401.15508069	-2401.1554524	-2403.28208251	-2403.30875883	-2403.30919805	-2403.30923549	-2403.30913436	-2403.30955048	-2403.31223482	-2403.31263138	-2403.31265223
B971	-2399.53557562	-2399.757518	-2399.77324411	-2399.7736059	-2401.91587766	-2401.94301386	-2401.94335969	-2401.94339186	-2401.94231237	-2401.94263928	-2401.94619442	-2401.94649946	-2401.94652019
HCTH	-2401.00656475	-2401.22420886	-2401.24067172	-2401.24104067	-2403.36579271	-2403.39357651	-2403.3942773	-2403.39431589	-2403.39377305	-2403.3944442	-2403.39705109	-2403.39769614	-2403.39772208
O3LYP	-2400.19237344	-2400.41238073	-2400.42884124	-2400.42920671	-2402.56533134	-2402.59294128	-2402.59364981	-2402.59369235	-2402.59244247	-2402.59313519	-2402.59602221	-2402.5967062	-2402.59673176
PBEPBE	-2399.31552836	-2399.54061472	-2399.55682633	-2399.55721389	-2401.68618215	-2401.71493711	-2401.71543964	-2401.7154766	-2401.71467831	-2401.7151611	-2401.71816963	-2401.71863432	-2401.7186576
tHCTHhybrid	-2399.85672489	-2400.07869549	-2400.09425877	-2400.09461389	-2402.22845307	-2402.25528752	-2402.25558449	-2402.25561987	-2402.25497439	-2402.25525324	-2402.25863253	-2402.25889099	-2402.25891146
QCISD/cc-pvtz	-2400.6701709												

S13c – Zero Point Vibrational Energy Corrections

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	0.005142	0.005507	0.005447	0.005391	0.005163	0.005362	0.005361	0.00536	0.005397	0.005395	0.005385	0.005386	0.005385
B3P86	0.005197	0.005589	0.005535	0.005492	0.005228	0.005435	0.005434	0.005433	0.005472	0.005471	0.005449	0.00545	0.00545
B3PW91	0.005186	0.005576	0.005522	0.005478	0.005227	0.005422	0.005421	0.00542	0.005457	0.005455	0.005441	0.005442	0.005441
B97D	0.005042	0.005356	0.005309	0.005255	0.005074	0.005237	0.005235	0.005235	0.00527	0.005268	0.005259	0.00526	0.005259
B971	0.005179	0.005557	0.005498	0.005443	0.005215	0.005401	0.0054	0.005399	0.005432	0.00543	0.005418	0.005418	0.005418
HCTH	0.005117	0.005503	0.005441	0.005386	0.005111	0.005312	0.00531	0.005309	0.00535	0.005346	0.005335	0.005335	0.005334
O3LYP	0.00518	0.005563	0.005507	0.005462	0.005184	0.005389	0.005387	0.005385	0.005425	0.005422	0.005407	0.005407	0.005406
PBEPBE	0.005057	0.005366	0.00531	0.005267	0.005098	0.005267	0.005266	0.005265	0.005299	0.005297	0.005275	0.005283	0.005283
tHCTHhybrid	0.005146	0.005531	0.005473	0.005417	0.005182	0.005373	0.005372	0.005371	0.005406	0.005404	0.005395	0.005396	0.005395
QCISD/cc-pVTZ	0.005645												

S14 – H.

S14a – Electronic Energies

	6-31G	6-31G(d,p)	6-31+G(d,p)	6-31++G(d,p)	6-311G	6-311G(d,p)	6-311+G(d,p)	6-311++G(d,p)	6-311G(2df,p)	6-311+G(2df,p)	6-311G(3df,3pd)	6-311+G(3df,3pd)	6-311++G(3df,3pd)
B3LYP	-0.500272784191	-0.500272784191	-0.500272784191	-0.501665908556	-0.50215593003	-0.502155930031	-0.502155930031	-0.502256981542	-0.502155930031	-0.502155930031	-0.502155930036	-0.502155930036	-0.502256981542
B3P86	-0.516817233085	-0.516817233085	-0.516817233085	-0.51792593661	-0.518515643862	-0.518515643862	-0.518515643862	-0.518572378951	-0.518515643862	-0.518515643862	-0.518515643867	-0.518515643867	-0.518572378964
B3PW91	-0.502176946479	-0.502176946479	-0.502176946479	-0.503376470334	-0.503978676903	-0.503978676904	-0.503978676904	-0.504065244241	-0.503978676904	-0.503978676904	-0.503978676908	-0.503978676908	-0.504065244255
B97D	-0.499978696516	-0.499978696516	-0.499978696516	-0.501409293564	-0.502455637312	-0.502455637312	-0.502455637312	-0.502842078908	-0.502455637312	-0.502455637312	-0.502455637313	-0.502455637313	-0.502842078908
B971	-0.500500435799	-0.500500435799	-0.500500435799	-0.501836853908	-0.502577796675	-0.502577796675	-0.502577796675	-0.502749690736	-0.502577796675	-0.502577796675	-0.502577796675	-0.502577796675	-0.502749690736
HCTH	-0.507752778946	-0.507752778946	-0.507752778946	-0.509136845575	-0.510025538527	-0.510025538528	-0.510025538528	-0.510289678264	-0.510025538528	-0.510025538528	-0.510025538528	-0.510025538528	-0.510289678264
O3LYP	-0.497340882376	-0.497340882376	-0.497340882376	-0.498897911345	-0.499582969602	-0.499582969602	-0.499582969602	-0.499836837658	-0.499582969602	-0.499582969602	-0.499582969603	-0.499582969603	-0.499836837658
PBEPBE	-0.497430908604	-0.497430908604	-0.497430908604	-0.499186653121	-0.499618064832	-0.499618064832	-0.499618064832	-0.49981227329	-0.499618064832	-0.499618064832	-0.499618064832	-0.499618064832	-0.49981227329
tHCTHhyb	-0.504997852503	-0.504997852503	-0.504997852503	-0.506258963658	-0.507084518748	-0.507084518748	-0.507084518748	-0.507306984054	-0.507084518748	-0.507084518748	-0.507084518749	-0.507084518749	-0.507306984054
QCISD/cc-pvtz	-0.4998098												