

Supporting Information

Physical Chemistry Chemical Physics

A larger basis set describes atomization energy core-valence correction better than a higher-order coupled-cluster method

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Extrapolation Techniques

In addition to using finite basis sets, we extrapolated the correlation energies to the complete basis set (CBS) limit using three different methods (**e1–e3**) as described below.

e1: The correlation energy is assumed to converge as $E_X = E + AX^{-3}$ (widely known as the Helgaker formula¹), where E_X stands for the correlation energy obtained with the basis set cardinal number X , E is the CBS limit energy, and A is a system-specific constant. The present formula was used for the two-point extrapolation of the total correlation energy for each considered coupled-cluster method.

e2: The following more flexible form was used: $E_X = E + AX^{-\beta}$, where β is a constant specific for a given pair of cardinal numbers, X and $X + 1$. Initially, this constant was derived for the two-point $2/3$ ($\beta = 2.46$) and $3/4$ ($\beta = 3.05$) extrapolations for the SD(T)/nZ level.² We optimized this exponent for the $4/5$ ($\beta = 3.22$) extrapolation by performing the $3/4/5$ three-point extrapolations for all available SD(T)/nZ ($n = T, Q, 5$) data and taking the median value. The described exponents were used for extrapolation of the SD- and SD(T)-level correlation energies. The higher-order increments were extrapolated separately using the same formula but specifically derived exponents: 2.7174 ($2/3$, SDT–SD(T)), 2.9968 ($2/3$, SDT(Q)–SDT), 1.7139 ($2/3$, SDTQ–SDT(Q)), 2.4807 ($3/4$, SDT–SD(T)), 3.3831 ($3/4$, SDT(Q)–SDT), and 2.6072 ($3/4$, SDT(Q)–SDT).³ There are no exponents optimized for higher contributions (SDTQ(P)–SDTQ and SDTQP–SDTQ(P)), so we assumed that these increments were sufficiently converged at the TZ level. The final extrapolated energy was then taken as the sum of the extrapolated SD(T)-level energies, extrapolated SDT–SD(T), SDT(Q)–SDT, and SDTQ–SDT(Q) increments (each with a specific exponent), and the SDTQP/TZ – SDTQ/TZ quantity. The extrapolations for the augmented basis sets were performed similarly, with the only difference in the $2/3$ exponent ($\beta = 2.51$) for the SD(T)/anZ level.²

e3: This is the recent extrapolation technique based on the Riemann zeta function.⁴ The key formula is $E = E_L + L^4(E_L - E_{L-1})\left(\frac{\pi^4}{90} - \sum_{l=1}^L l^{-4}\right)$, where E_L is the correlation energy obtained with the basis set cardinal number L , and E is the exact energy. This two-point extrapolation method does not require the

determination of any additional L-specific constants. This technique was applied to the full correlation energies for each considered coupled-cluster method, as in the **e1** method.

For clarity, the abbreviation “eN{X,Y}Z” was used throughout the text, where eN represents the type of the two-point extrapolation (**e1–e3**), while XZ and YZ are two consecutive basis sets used for this extrapolation.

The extrapolated energies can be represented as a linear combination of finite basis set energies in all cases (**e1–e3**). Therefore, when the reaction energies are of interest (e.g. total atomization energy), there is no difference in whether they are extrapolated directly or the energies of the individual systems are extrapolated first and then subtracted.

The extrapolation of the Hartree-Fock energy was performed similarly for all methods (**e1–e3**) by using $E_X = E + A \exp(-\alpha X^{1/2})$ formula with fitted values of α (4.42 for 2/3 and 5.46 for 3/4 extrapolation).²

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2. F. Neese and E. F. Valeev, *J. Chem. Theory Comput.*, 2011, **7**, 33-43. DOI: 10.1021/ct100396y
3. A. Karton, *J. Chem. Phys.*, 2020, **153**, 024102. DOI: 10.1063/5.0011674
4. M. Lesiuk and B. Jeziorski, *J. Chem. Theory Comput.*, 2019, **15**, 5398-5403. DOI: 10.1021/acs.jctc.9b00705

Batch #1

Table S1. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SD(T)/eN{Q,5}Z (N = 1 – 3) values. The range of SD(T)/eN{Q,5}Z (N = 1 – 3) values (RANGE, RMS = 0.0094 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SD/DZ	SD(T)/DZ	SD/TZ	SD(T)/TZ	SD/QZ	SD(T)/QZ	SD/SZ	SD(T)/SZ	SD/e{D,T}Z	SD(T)/e{D,T}Z	SD/e{T,Q}Z	SD(T)/e{T,Q}Z	SD/e{Q,5}Z	SD(T)/e{Q,5}Z	SD/e2{D,T}Z	SD(T)/e2{D,T}Z	SD/e2{T,Q}Z	SD(T)/e2{T,Q}Z	SD/e2{Q,5}Z	SD(T)/e2{Q,5}Z	SD/e3{D,T}Z	SD(T)/e3{D,T}Z	SD/e3{T,Q}Z	SD(T)/e3{T,Q}Z	SD/e3{Q,5}Z	SD(T)/e3{Q,5}Z
alcl	0.4094	0.0028	0.3314	0.1827	0.2214	0.0584	0.1970	0.0205	0.1920	0.0106	0.1751	0.0060	0.1791	0.0072	0.1867	0.0003	0.1572	0.0143	0.1795	0.0065	0.1872	0.0012	0.1548	0.0169	0.1746	0.0142	0.1858	0.0015
alf	0.6198	0.0207	0.8341	0.7601	0.4254	0.3311	0.2663	0.1527	0.2005	0.0792	0.2533	0.1504	0.1501	0.0225	0.1316	0.0021	0.1866	0.0803	0.1530	0.0257	0.1380	0.0093	0.1779	0.0712	0.1208	0.0104	0.1196	0.0114
alh	-0.1010	0.0011	0.2440	0.1564	0.1318	0.0327	0.1176	0.0079	0.1174	0.0041	0.0845	0.0193	0.1073	0.0102	0.1171	0.0001	0.0662	0.0395	0.1076	0.0098	0.1172	0.0005	0.0638	0.0422	0.1047	0.0148	0.1171	0.0006
alh3	-0.6714	0.0053	0.6728	0.7693	0.1474	0.1275	0.2550	0.0392	0.2785	0.0203	0.4927	0.1428	0.3335	0.0253	0.3031	0.0005	0.6266	0.2476	0.3316	0.0237	0.3008	0.0024	0.6441	0.2613	0.3533	0.0415	0.3074	0.0029
bf	0.7881	0.0073	0.3949	0.3732	0.2065	0.1515	0.1167	0.0541	0.0927	0.0280	0.1272	0.0582	0.0512	0.0171	0.0674	0.0007	0.0964	0.0220	0.0528	0.0153	0.0698	0.0033	0.0924	0.0172	0.0346	0.0350	0.0630	0.0040
bh	0.2136	0.0013	0.1562	0.1216	0.0828	0.0287	0.0687	0.0100	0.0653	0.0052	0.0519	0.0105	0.0585	0.0037	0.0616	0.0001	0.0399	0.0256	0.0587	0.0033	0.0620	0.0006	0.0383	0.0276	0.0559	0.0071	0.0610	0.0007
bh3	1.1503	0.0073	0.6194	0.6718	0.0691	0.1552	0.0327	0.0540	0.0588	0.0280	0.1625	0.0623	0.1071	0.0199	0.0861	0.0007	0.2524	0.1467	0.1053	0.0181	0.0835	0.0033	0.2641	0.1577	0.1259	0.0386	0.0908	0.0040
c2h2	2.6228	0.0170	1.2407	1.1681	0.4994	0.3403	0.3077	0.1256	0.2536	0.0651	0.1872	0.0083	0.1678	0.0311	0.1970	0.0017	0.0662	0.1434	0.1712	0.0273	0.2023	0.0076	0.0504	0.1611	0.1324	0.0708	0.1871	0.0093
c2h3f	2.6234	0.0141	0.9827	0.8940	0.4639	0.2802	0.3134	0.1044	0.2704	0.0541	0.2454	0.0218	0.2037	0.0240	0.2252	0.0014	0.1607	0.0784	0.2063	0.0208	0.2295	0.0063	0.1497	0.0915	0.1759	0.0564	0.2174	0.0078
c2h4	2.5094	0.0140	1.0144	0.9581	0.3947	0.2807	0.2352	0.1034	0.1904	0.0536	0.1337	0.0045	0.1188	0.0260	0.1434	0.0014	0.0325	0.1152	0.1217	0.0229	0.1478	0.0063	0.0193	0.1296	0.0894	0.0588	0.1352	0.0077
ccl2	0.7729	0.0027	0.3955	0.0416	0.3709	0.1033	0.4873	0.0198	0.5091	0.0103	0.3606	0.1643	0.5722	0.0411	0.5321	0.0003	0.3566	0.1880	0.5701	0.0396	0.5299	0.0012	0.3561	0.1911	0.5936	0.0565	0.5361	0.0015
cf2	0.6058	0.0018	0.0594	0.0328	0.2261	0.0368	0.2215	0.0134	0.2201	0.0069	0.2963	0.0661	0.2182	0.0037	0.2185	0.0002	0.3236	0.0775	0.2182	0.0033	0.2187	0.0008	0.3271	0.0790	0.2173	0.0080	0.2183	0.0010
ch2c	1.9148	0.0117	0.8770	0.8038	0.3773	0.2357	0.2470	0.0864	0.2109	0.0448	0.1670	0.0035	0.1520	0.0225	0.1729	0.0012	0.0854	0.0962	0.1543	0.0199	0.1765	0.0053	0.0747	0.1084	0.1279	0.0501	0.1663	0.0064
ch2nh	1.8027	0.0098	0.6593	0.5588	0.3861	0.1931	0.2878	0.0725	0.2593	0.0376	0.2711	0.0392	0.2161	0.0155	0.2294	0.0010	0.2265	0.0205	0.2179	0.0133	0.2322	0.0044	0.2206	0.0283	0.1980	0.0377	0.2241	0.0054
ch2-sing	0.4607	0.0023	0.1780	0.1288	0.1226	0.0483	0.0976	0.0172	0.0909	0.0089	0.0993	0.0144	0.0794	0.0054	0.0839	0.0002	0.0903	0.0012	0.0798	0.0048	0.0845	0.0010	0.0891	0.0005	0.0748	0.0111	0.0827	0.0013
ch3f	1.2829	0.0060	0.3548	0.3151	0.2026	0.1191	0.1412	0.0447	0.1236	0.0232	0.1385	0.0365	0.0963	0.0097	0.1052	0.0006	0.1137	0.0045	0.0974	0.0083	0.1069	0.0027	0.1104	0.0003	0.0850	0.0234	0.1020	0.0033
ch3nh2	1.9726	0.0092	0.5619	0.4953	0.3085	0.1815	0.2133	0.0683	0.1861	0.0354	0.2018	0.0494	0.1438	0.0144	0.1576	0.0009	0.1604	0.0019	0.1455	0.0124	0.1603	0.0042	0.1550	0.0086	0.1262	0.0353	0.1527	0.0051
ch4	1.3312	0.0071	0.4661	0.4590	0.1590	0.1446	0.0728	0.0526	0.0492	0.0273	0.0296	0.0122	0.0099	0.0145	0.0243	0.0007	0.0205	0.0392	0.0115	0.0128	0.0267	0.0032	0.0271	0.0459	0.0060	0.0314	0.0200	0.0039
c-hcoh	0.9832	0.0049	0.2822	0.2040	0.2471	0.0937	0.2058	0.0363	0.1928	0.0188	0.2324	0.0473	0.1757	0.0057	0.1791	0.0005	0.2267	0.0293	0.1764	0.0047	0.1804	0.0022	0.2259	0.0270	0.1680	0.0163	0.1767	0.0027
c-hono	0.8667	0.0030	0.1439	0.0583	0.4325	0.0440	0.4476	0.0220	0.4472	0.0114	0.5540	0.0870	0.4587	0.0059	0.4468	0.0003	0.6012	0.1037	0.4584	0.0063	0.4468	0.0013	0.6073	0.1059	0.4615	0.0018	0.4467	0.0016

System	REFERENCE	RANGE	SD/DZ	SD(T)/DZ	SD/TZ	SD(T)/TZ	SD/QZ	SD(T)/QZ	SD/5Z	SD(T)/5Z	SD/e1{D,T}Z	SD(T)/e1{D,T}Z	SD/e1{T,Q}Z	SD(T)/e1{T,Q}Z	SD/e1{Q,5}Z	SD(T)/e1{Q,5}Z	SD/e2{D,T}Z	SD(T)/e2{D,T}Z	SD/e2{T,Q}Z	SD(T)/e2{T,Q}Z	SD/e2{Q,5}Z	SD(T)/e2{Q,5}Z	SD/e3{D,T}Z	SD(T)/e3{D,T}Z	SD/e3{T,Q}Z	SD(T)/e3{T,Q}Z	SD/e3{Q,5}Z	SD(T)/e3{Q,5}Z
cl2	0.2572	0.0066	0.2385	0.0492	0.2556	0.1274	0.3600	0.0488	0.3920	0.0253	0.2628	0.1603	0.4362	0.0086	0.4255	0.0007	0.2656	0.1731	0.4343	0.0072	0.4224	0.0030	0.2660	0.1748	0.4555	0.0231	0.4314	0.0036
clcn	2.0616	0.0088	0.9346	0.6869	0.5397	0.1525	0.4874	0.0653	0.4672	0.0339	0.3734	0.0726	0.4493	0.0017	0.4460	0.0009	0.3089	0.1598	0.4503	0.0033	0.4480	0.0040	0.3005	0.1712	0.4397	0.0143	0.4424	0.0049
clf	0.1399	0.0048	0.0716	0.1146	0.1794	0.0803	0.2449	0.0353	0.2691	0.0183	0.2247	0.0659	0.2927	0.0025	0.2945	0.0005	0.2423	0.0603	0.2915	0.0033	0.2922	0.0021	0.2446	0.0596	0.3048	0.0058	0.2990	0.0026
c-n2h2	0.9857	0.0045	0.2809	0.1242	0.3721	0.0823	0.3501	0.0331	0.3417	0.0171	0.4105	0.0646	0.3340	0.0029	0.3330	0.0004	0.4254	0.0578	0.3343	0.0020	0.3338	0.0020	0.4274	0.0569	0.3299	0.0120	0.3315	0.0025
co	1.1318	0.0094	0.5711	0.4902	0.3567	0.1798	0.2669	0.0694	0.2393	0.0360	0.2664	0.0491	0.2014	0.0112	0.2103	0.0009	0.2314	0.0016	0.2030	0.0092	0.2130	0.0042	0.2269	0.0082	0.1848	0.0316	0.2052	0.0052
co2	2.0468	0.0145	0.8292	0.6975	0.5492	0.2717	0.4174	0.1072	0.3750	0.0556	0.4313	0.0923	0.3213	0.0128	0.3306	0.0015	0.3855	0.0228	0.3236	0.0099	0.3348	0.0065	0.3796	0.0137	0.2970	0.0431	0.3229	0.0080
cs	1.0464	0.0085	0.8685	0.5534	0.5726	0.1270	0.5516	0.0628	0.5364	0.0326	0.4480	0.0525	0.5363	0.0159	0.5205	0.0009	0.3997	0.1221	0.5366	0.0171	0.5220	0.0038	0.3934	0.1312	0.5324	0.0041	0.5178	0.0047
cs2	1.9868	0.0056	1.2520	0.7727	0.7141	0.0961	0.7143	0.0414	0.7132	0.0215	0.4877	0.1888	0.7144	0.0014	0.7120	0.0006	0.3999	0.2993	0.7144	0.0024	0.7121	0.0025	0.3884	0.3138	0.7144	0.0087	0.7118	0.0031
dioxirane	1.4135	0.0050	0.3442	0.1689	0.4329	0.0938	0.4118	0.0372	0.4041	0.0193	0.4703	0.0622	0.3964	0.0042	0.3959	0.0005	0.4848	0.0499	0.3968	0.0032	0.3967	0.0023	0.4867	0.0483	0.3925	0.0146	0.3945	0.0028
f2	0.0084	0.0010	0.0286	0.1017	0.2119	0.0197	0.2436	0.0075	0.2525	0.0039	0.2891	0.0148	0.2667	0.0013	0.2618	0.0001	0.3190	0.0282	0.2661	0.0011	0.2609	0.0005	0.3229	0.0300	0.2725	0.0036	0.2635	0.0006
f2co	1.7404	0.0095	0.4817	0.3433	0.4634	0.1783	0.3877	0.0704	0.3628	0.0365	0.4558	0.1088	0.3324	0.0084	0.3366	0.0010	0.4528	0.0818	0.3338	0.0064	0.3390	0.0043	0.4524	0.0783	0.3185	0.0283	0.3320	0.0052
fccf	3.1610	0.0186	1.3257	1.1791	0.6760	0.3674	0.4842	0.1375	0.4287	0.0713	0.4025	0.0256	0.3442	0.0303	0.3705	0.0019	0.2964	0.1069	0.3477	0.0262	0.3759	0.0084	0.2825	0.1242	0.3088	0.0728	0.3604	0.0102
formic	1.9196	0.0107	0.5935	0.4715	0.4479	0.2009	0.3548	0.0792	0.3248	0.0411	0.3866	0.0870	0.2868	0.0096	0.2933	0.0011	0.3629	0.0428	0.2885	0.0074	0.2963	0.0048	0.3598	0.0370	0.2696	0.0321	0.2879	0.0059
h2co	1.4753	0.0087	0.5545	0.4675	0.3421	0.1685	0.2582	0.0644	0.2328	0.0334	0.2527	0.0426	0.1969	0.0115	0.2062	0.0009	0.2180	0.0062	0.1984	0.0096	0.2087	0.0039	0.2134	0.0126	0.1814	0.0307	0.2016	0.0048
h2o	0.4768	0.0022	0.0988	0.0661	0.1027	0.0414	0.0843	0.0159	0.0793	0.0083	0.1043	0.0311	0.0709	0.0027	0.0741	0.0002	0.1049	0.0271	0.0713	0.0023	0.0745	0.0010	0.1050	0.0265	0.0675	0.0074	0.0731	0.0012
h2s	0.4455	0.0008	0.3051	0.1791	0.1060	0.0223	0.1314	0.0061	0.1376	0.0032	0.0222	0.1070	0.1499	0.0056	0.1441	0.0001	0.0104	0.1399	0.1495	0.0053	0.1435	0.0004	0.0146	0.1442	0.1546	0.0086	0.1453	0.0005
hccf	2.8756	0.0179	1.2694	1.1615	0.5853	0.3539	0.3942	0.1325	0.3389	0.0687	0.2972	0.0138	0.2548	0.0290	0.2808	0.0018	0.1855	0.1181	0.2582	0.0250	0.2862	0.0081	0.1709	0.1353	0.2195	0.0698	0.2707	0.0099
hcl	0.2675	0.0005	0.1560	0.0855	0.0755	0.0010	0.0837	0.0036	0.0833	0.0019	0.0416	0.0374	0.0897	0.0070	0.0828	0.0000	0.0284	0.0515	0.0896	0.0069	0.0829	0.0002	0.0267	0.0533	0.0912	0.0078	0.0827	0.0003
hcn	1.8806	0.0133	0.9066	0.7913	0.4971	0.2626	0.3609	0.0986	0.3212	0.0511	0.3248	0.0400	0.2614	0.0211	0.2795	0.0013	0.2579	0.0463	0.2639	0.0181	0.2834	0.0060	0.2492	0.0576	0.2363	0.0513	0.2723	0.0073
hcno	2.5758	0.0150	0.9922	0.8035	0.6698	0.2915	0.5321	0.1112	0.4904	0.0577	0.5340	0.0759	0.4315	0.0204	0.4467	0.0015	0.4814	0.0077	0.4340	0.0172	0.4508	0.0068	0.4745	0.0186	0.4061	0.0537	0.4391	0.0083
hf	0.2317	0.0009	0.0499	0.0325	0.0526	0.0169	0.0470	0.0067	0.0455	0.0035	0.0537	0.0104	0.0430	0.0008	0.0438	0.0001	0.0541	0.0078	0.0431	0.0006	0.0440	0.0004	0.0542	0.0075	0.0420	0.0027	0.0435	0.0005
hnc	1.6505	0.0110	0.7173	0.6230	0.4150	0.2181	0.3013	0.0813	0.2686	0.0422	0.2877	0.0476	0.2183	0.0185	0.2343	0.0011	0.2384	0.0185	0.2203	0.0161	0.2376	0.0049	0.2319	0.0271	0.1973	0.0438	0.2284	0.0061
hnco	2.4516	0.0156	0.9358	0.7924	0.5930	0.3000	0.4430	0.1153	0.3974	0.0598	0.4487	0.0926	0.3336	0.0195	0.3496	0.0016	0.3927	0.0122	0.3363	0.0162	0.3540	0.0070	0.3854	0.0017	0.3060	0.0536	0.3412	0.0086
hnnn	1.8891	0.0100	0.6455	0.4078	0.6454	0.1888	0.5770	0.0736	0.5545	0.0382	0.6453	0.0967	0.5270	0.0105	0.5310	0.0010	0.6453	0.0609	0.5283	0.0084	0.5332	0.0045	0.6453	0.0562	0.5144	0.0317	0.5269	0.0055
hno	0.6472	0.0024	0.1733	0.0200	0.3275	0.0425	0.3292	0.0181	0.3276	0.0094	0.3925	0.0519	0.3303	0.0003	0.3260	0.0002	0.4177	0.0556	0.3303	0.0007	0.3262	0.0011	0.4209	0.0561	0.3306	0.0042	0.3257	0.0013
hocl	0.4234	0.0027	0.1376	0.0599	0.2385	0.0487	0.2924	0.0200	0.3107	0.0104	0.2810	0.0440	0.3317	0.0010	0.3298	0.0003	0.2975	0.0422	0.3308	0.0004	0.3281	0.0012	0.2996	0.0419	0.3417	0.0063	0.3332	0.0015
hocn	2.3552	0.0150	0.9448	0.7859	0.6066	0.2874	0.4662	0.1108	0.4229	0.0575	0.4642	0.0774	0.3637	0.0180	0.3776	0.0015	0.4090	0.0040	0.3662	0.0149	0.3818	0.0067	0.4018	0.0146	0.3377	0.0506	0.3697	0.0082
hof	0.2667	0.0001	0.0293	0.0838	0.2120	0.0011	0.2314	0.0008	0.2368	0.0004	0.2889	0.0369	0.2456	0.0005	0.2424	0.0000	0.3188	0.0507	0.2453	0.0005	0.2419	0.0000	0.3227	0.0525	0.2492	0.0005	0.2434	0.0001

System	REFERENCE	RANGE	SD/DZ	SD(T)/DZ	SD/TZ	SD(T)/TZ	SD/QZ	SD(T)/QZ	SD/5Z	SD(T)/5Z	SD/e1{D,T}Z	SD(T)/e1{D,T}Z	SD/e1{T,Q}Z	SD(T)/e1{T,Q}Z	SD/e1{Q,5}Z	SD(T)/e1{Q,5}Z	SD/e2{D,T}Z	SD(T)/e2{D,T}Z	SD/e2{T,Q}Z	SD(T)/e2{T,Q}Z	SD/e2{Q,5}Z	SD(T)/e2{Q,5}Z	SD/e3{D,T}Z	SD(T)/e3{D,T}Z	SD/e3{T,Q}Z	SD(T)/e3{T,Q}Z	SD/e3{Q,5}Z	SD(T)/e3{Q,5}Z
honc	1.9160	0.0113	0.6991	0.5365	0.5449	0.2142	0.4499	0.0832	0.4198	0.0431	0.4800	0.0784	0.3805	0.0124	0.3883	0.0011	0.4548	0.0258	0.3822	0.0100	0.3913	0.0051	0.4515	0.0189	0.3630	0.0365	0.3828	0.0062
hooh	0.5601	0.0016	0.0731	0.0406	0.2445	0.0279	0.2503	0.0120	0.2512	0.0062	0.3166	0.0567	0.2545	0.0004	0.2521	0.0002	0.3446	0.0679	0.2544	0.0007	0.2520	0.0007	0.3483	0.0694	0.2555	0.0025	0.2523	0.0009
ketene	2.9891	0.0184	1.2148	1.1053	0.5886	0.3585	0.3974	0.1363	0.3405	0.0707	0.3250	0.0440	0.2578	0.0258	0.2808	0.0019	0.2228	0.0779	0.2612	0.0219	0.2864	0.0083	0.2094	0.0938	0.2225	0.0668	0.2704	0.0101
methanol	1.5946	0.0076	0.4378	0.3819	0.2588	0.1473	0.1839	0.0564	0.1617	0.0293	0.1834	0.0486	0.1292	0.0099	0.1384	0.0008	0.1542	0.0102	0.1305	0.0083	0.1406	0.0034	0.1504	0.0052	0.1154	0.0267	0.1344	0.0042
n2	1.0684	0.0080	0.5449	0.3931	0.4504	0.1543	0.3865	0.0594	0.3667	0.0308	0.4106	0.0537	0.3399	0.0099	0.3460	0.0008	0.3952	0.0147	0.3410	0.0082	0.3480	0.0036	0.3932	0.0096	0.3281	0.0274	0.3424	0.0044
n2h4	1.3939	0.0054	0.2925	0.1827	0.3108	0.1062	0.2674	0.0400	0.2554	0.0208	0.3185	0.0740	0.2357	0.0082	0.2428	0.0005	0.3214	0.0615	0.2364	0.0071	0.2440	0.0024	0.3218	0.0599	0.2277	0.0204	0.2406	0.0030
n2o	1.5454	0.0086	0.5151	0.2842	0.6045	0.1551	0.5584	0.0636	0.5401	0.0330	0.6421	0.1007	0.5247	0.0031	0.5210	0.0009	0.6567	0.0796	0.5255	0.0014	0.5228	0.0039	0.6587	0.0769	0.5162	0.0199	0.5176	0.0047
nccn	3.8062	0.0259	1.7242	1.4751	0.9992	0.5018	0.7465	0.1916	0.6706	0.0994	0.6939	0.0920	0.5621	0.0348	0.5910	0.0026	0.5755	0.0669	0.5666	0.0292	0.5984	0.0117	0.5600	0.0877	0.5155	0.0920	0.5771	0.0143
nh2cl	0.7528	0.0004	0.2178	0.0303	0.2629	0.0140	0.2990	0.0030	0.3091	0.0016	0.2819	0.0326	0.3254	0.0050	0.3197	0.0000	0.2892	0.0399	0.3247	0.0048	0.3187	0.0002	0.2902	0.0408	0.3320	0.0070	0.3215	0.0002
nh3	0.7791	0.0035	0.1817	0.1363	0.1520	0.0717	0.1153	0.0258	0.1061	0.0134	0.1396	0.0445	0.0886	0.0077	0.0964	0.0004	0.1347	0.0340	0.0892	0.0069	0.0973	0.0016	0.1341	0.0326	0.0818	0.0162	0.0947	0.0019
ocs	2.0202	0.0109	1.0173	0.7462	0.5864	0.1881	0.5193	0.0809	0.4935	0.0419	0.4049	0.0468	0.4704	0.0026	0.4664	0.0011	0.3345	0.1380	0.4716	0.0045	0.4690	0.0049	0.3253	0.1499	0.4580	0.0172	0.4617	0.0060
oxirene	2.6280	0.0126	1.0132	0.8623	0.5693	0.2592	0.4407	0.0933	0.4065	0.0484	0.3823	0.0052	0.3469	0.0277	0.3706	0.0013	0.3098	0.0932	0.3492	0.0247	0.3739	0.0057	0.3004	0.1061	0.3232	0.0583	0.3643	0.0069
p2	0.9716	0.0004	1.0739	0.3914	0.8788	0.0054	0.9434	0.0030	0.9654	0.0016	0.7967	0.1571	0.9906	0.0092	0.9885	0.0000	0.7649	0.2202	0.9894	0.0090	0.9863	0.0002	0.7607	0.2284	1.0025	0.0107	0.9925	0.0002
ph3	0.4547	0.0044	0.3889	0.2420	0.0813	0.0559	0.1227	0.0326	0.1444	0.0169	0.0482	0.1814	0.1529	0.0155	0.1671	0.0004	0.0985	0.2300	0.1521	0.0159	0.1650	0.0020	0.1050	0.2364	0.1605	0.0112	0.1711	0.0024
sih3f	0.1712	0.0046	0.8794	0.8505	0.1181	0.1771	0.0167	0.0341	0.0281	0.0177	0.2025	0.1064	0.1150	0.0704	0.0401	0.0005	0.3268	0.2164	0.1126	0.0678	0.0390	0.0021	0.3431	0.2307	0.1398	0.0968	0.0422	0.0025
sih4	-0.0259	0.0020	0.7742	0.7605	0.0379	0.0649	0.1200	0.0149	0.1118	0.0077	0.3798	0.2280	0.1798	0.0731	0.1032	0.0002	0.5124	0.3416	0.1784	0.0717	0.1040	0.0009	0.5298	0.3564	0.1950	0.0878	0.1017	0.0011
sio	1.1827	0.0207	1.1245	0.9235	0.6351	0.3571	0.4651	0.1534	0.4037	0.0795	0.4290	0.1186	0.3411	0.0047	0.3393	0.0021	0.3491	0.0261	0.3442	0.0084	0.3454	0.0093	0.3387	0.0140	0.3098	0.0329	0.3281	0.0114
so2	1.2417	0.0020	0.7633	0.4062	0.5762	0.0507	0.5975	0.0147	0.6109	0.0076	0.4974	0.0989	0.6131	0.0116	0.6248	0.0002	0.4668	0.1570	0.6127	0.0110	0.6235	0.0009	0.4628	0.1646	0.6171	0.0183	0.6273	0.0011
t-hcoh	1.0322	0.0049	0.3017	0.2260	0.2465	0.0966	0.2024	0.0364	0.1892	0.0189	0.2233	0.0421	0.1702	0.0075	0.1755	0.0005	0.2142	0.0210	0.1709	0.0065	0.1767	0.0022	0.2131	0.0182	0.1620	0.0186	0.1731	0.0027
t-hono	0.8783	0.0027	0.1549	0.0520	0.4402	0.0419	0.4564	0.0199	0.4574	0.0103	0.5603	0.0814	0.4683	0.0038	0.4585	0.0003	0.6069	0.0967	0.4680	0.0042	0.4584	0.0012	0.6130	0.0987	0.4713	0.0002	0.4587	0.0015
t-n2h2	1.0306	0.0044	0.2946	0.1412	0.3696	0.0842	0.3450	0.0322	0.3374	0.0167	0.4011	0.0602	0.3270	0.0058	0.3293	0.0004	0.4134	0.0509	0.3275	0.0049	0.3301	0.0020	0.4150	0.0497	0.3225	0.0154	0.3279	0.0024
cch	2.2462	0.0148	1.1555	1.0685	0.4768	0.2999	0.3093	0.1092	0.2632	0.0567	0.1911	0.0237	0.1871	0.0299	0.2149	0.0015	0.0803	0.1492	0.1900	0.0265	0.2194	0.0066	0.0658	0.1656	0.1561	0.0650	0.2064	0.0081
cf	0.4154	0.0018	0.1125	0.0657	0.1372	0.0384	0.1215	0.0130	0.1178	0.0067	0.1476	0.0269	0.1101	0.0056	0.1140	0.0002	0.1516	0.0225	0.1104	0.0051	0.1143	0.0008	0.1521	0.0219	0.1072	0.0103	0.1133	0.0010
ch	0.1831	0.0007	0.0634	0.0342	0.0640	0.0164	0.0573	0.0055	0.0560	0.0028	0.0642	0.0089	0.0525	0.0025	0.0546	0.0001	0.0643	0.0060	0.0526	0.0024	0.0547	0.0003	0.0643	0.0057	0.0513	0.0046	0.0544	0.0004
ch2ch	2.3096	0.0132	0.9871	0.9352	0.3703	0.2665	0.2179	0.0974	0.1758	0.0505	0.1106	0.0150	0.1067	0.0260	0.1316	0.0013	0.0099	0.1242	0.1094	0.0230	0.1358	0.0059	0.0033	0.1385	0.0785	0.0572	0.1240	0.0072
ch2nh2	1.9804	0.0089	0.6256	0.5656	0.3021	0.1848	0.1999	0.0656	0.1737	0.0340	0.1659	0.0244	0.1253	0.0214	0.1461	0.0009	0.1131	0.0377	0.1271	0.0193	0.1487	0.0040	0.1062	0.0459	0.1064	0.0434	0.1413	0.0049
ch3	1.1186	0.0059	0.4214	0.4236	0.1224	0.1234	0.0469	0.0437	0.0273	0.0227	0.0035	0.0030	0.0082	0.0145	0.0067	0.0006	0.0524	0.0520	0.0069	0.0130	0.0086	0.0027	0.0588	0.0584	0.0222	0.0292	0.0031	0.0033
ch3nh	1.6877	0.0079	0.4965	0.4375	0.2704	0.1567	0.1889	0.0587	0.1659	0.0304	0.1753	0.0385	0.1294	0.0129	0.1417	0.0008	0.1383	0.0074	0.1309	0.0111	0.1440	0.0036	0.1335	0.0134	0.1144	0.0310	0.1375	0.0044

System	REFERENCE	RANGE	SD/DZ	SD(T)/DZ	SD/TZ	SD(T)/TZ	SD/QZ	SD(T)/QZ	SD/5Z	SD(T)/5Z	SD/e1{D,T}Z	SD(T)/e1{D,T}Z	SD/e1{T,Q}Z	SD(T)/e1{T,Q}Z	SD/e1{Q,5}Z	SD(T)/e1{Q,5}Z	SD/e2{D,T}Z	SD(T)/e2{D,T}Z	SD/e2{T,Q}Z	SD(T)/e2{T,Q}Z	SD/e2{Q,5}Z	SD(T)/e2{Q,5}Z	SD/e3{D,T}Z	SD(T)/e3{D,T}Z	SD/e3{T,Q}Z	SD(T)/e3{T,Q}Z	SD/e3{Q,5}Z	SD(T)/e3{Q,5}Z
clo	0.3081	0.0044	0.1733	0.0365	0.2557	0.0660	0.3226	0.0324	0.3502	0.0168	0.2904	0.0784	0.3714	0.0079	0.3792	0.0004	0.3039	0.0833	0.3702	0.0085	0.3765	0.0020	0.3056	0.0839	0.3838	0.0017	0.3842	0.0024
cn	1.4216	0.0299	0.8487	0.6861	0.6344	0.3707	0.4944	0.2213	0.3903	0.1148	0.5441	0.2378	0.3923	0.1123	0.2810	0.0030	0.5091	0.1863	0.3948	0.1150	0.2913	0.0135	0.5046	0.1796	0.3665	0.0848	0.2620	0.0165
h2cn	1.6636	0.0097	0.6847	0.5867	0.3794	0.1926	0.2805	0.0719	0.2522	0.0373	0.2508	0.0267	0.2084	0.0162	0.2225	0.0010	0.2009	0.0376	0.2102	0.0141	0.2253	0.0044	0.1944	0.0460	0.1902	0.0385	0.2173	0.0054
hcnh	1.6982	0.0095	0.6826	0.5856	0.3828	0.1923	0.2828	0.0702	0.2553	0.0364	0.2566	0.0267	0.2098	0.0189	0.2265	0.0010	0.2076	0.0376	0.2116	0.0168	0.2292	0.0043	0.2012	0.0460	0.1914	0.0415	0.2215	0.0052
hco	1.3271	0.0085	0.5679	0.4919	0.3311	0.1681	0.2456	0.0629	0.2208	0.0326	0.2314	0.0317	0.1832	0.0138	0.1949	0.0009	0.1927	0.0212	0.1847	0.0119	0.1973	0.0038	0.1876	0.0281	0.1674	0.0332	0.1904	0.0047
hoo	0.4157	0.0008	0.0547	0.0483	0.2108	0.0110	0.2247	0.0057	0.2272	0.0030	0.2765	0.0360	0.2349	0.0018	0.2298	0.0001	0.3020	0.0457	0.2347	0.0019	0.2295	0.0003	0.3054	0.0470	0.2375	0.0008	0.2302	0.0004
hs	0.2276	0.0003	0.1425	0.0768	0.0526	0.0134	0.0699	0.0019	0.0728	0.0010	0.0148	0.0514	0.0825	0.0065	0.0758	0.0000	0.0001	0.0661	0.0822	0.0063	0.0755	0.0001	0.0018	0.0680	0.0857	0.0087	0.0763	0.0001
n2h	1.0384	0.0055	0.3914	0.2460	0.3827	0.1080	0.3431	0.0409	0.3312	0.0212	0.3791	0.0499	0.3142	0.0081	0.3187	0.0006	0.3777	0.0274	0.3149	0.0069	0.3199	0.0025	0.3775	0.0244	0.3069	0.0205	0.3165	0.0030
nh2	0.4227	0.0018	0.0765	0.0396	0.1041	0.0370	0.0881	0.0133	0.0845	0.0069	0.1157	0.0359	0.0764	0.0041	0.0807	0.0002	0.1202	0.0355	0.0767	0.0036	0.0811	0.0008	0.1208	0.0355	0.0735	0.0085	0.0801	0.0010
no	0.6262	0.0033	0.2319	0.1016	0.3113	0.0598	0.3006	0.0242	0.2957	0.0126	0.3448	0.0423	0.2927	0.0018	0.2907	0.0003	0.3577	0.0354	0.2929	0.0012	0.2912	0.0015	0.3594	0.0345	0.2907	0.0084	0.2898	0.0018
no2	1.0139	0.0038	0.2443	0.0424	0.4561	0.0621	0.4619	0.0280	0.4593	0.0145	0.5453	0.0703	0.4661	0.0032	0.4565	0.0004	0.5798	0.0735	0.4660	0.0038	0.4568	0.0017	0.5844	0.0739	0.4672	0.0031	0.4561	0.0021
oh	0.2025	0.0008	0.0307	0.0101	0.0549	0.0152	0.0500	0.0057	0.0490	0.0029	0.0651	0.0174	0.0464	0.0013	0.0478	0.0001	0.0691	0.0183	0.0465	0.0012	0.0479	0.0003	0.0696	0.0184	0.0455	0.0031	0.0476	0.0004
sif	0.4928	0.0090	0.3769	0.3114	0.2382	0.1532	0.1693	0.0663	0.1441	0.0344	0.1798	0.0866	0.1190	0.0029	0.1177	0.0009	0.1572	0.0608	0.1203	0.0044	0.1201	0.0040	0.1542	0.0574	0.1063	0.0132	0.1130	0.0049
sih	0.0274	0.0006	0.1542	0.0839	0.0673	0.0032	0.0751	0.0044	0.0803	0.0023	0.0307	0.0399	0.0808	0.0052	0.0858	0.0001	0.0165	0.0541	0.0807	0.0052	0.0853	0.0003	0.0147	0.0560	0.0823	0.0054	0.0868	0.0003
ssh	0.6532	0.0063	0.4636	0.1341	0.2604	0.1390	0.3844	0.0463	0.4163	0.0240	0.1748	0.2540	0.4749	0.0214	0.4498	0.0006	0.1416	0.2986	0.4727	0.0198	0.4466	0.0028	0.1372	0.3045	0.4978	0.0386	0.4556	0.0034
ch2-trip	0.8449	0.0047	0.3538	0.3714	0.0714	0.0998	0.0077	0.0349	0.0084	0.0181	0.0475	0.0146	0.0388	0.0125	0.0252	0.0005	0.0936	0.0589	0.0376	0.0114	0.0236	0.0021	0.0996	0.0647	0.0505	0.0245	0.0282	0.0026
nh	0.1644	0.0005	0.0122	0.0093	0.0517	0.0112	0.0489	0.0037	0.0489	0.0019	0.0684	0.0198	0.0469	0.0018	0.0488	0.0001	0.0748	0.0232	0.0469	0.0016	0.0488	0.0002	0.0757	0.0236	0.0464	0.0032	0.0487	0.0003
o2	0.3716	0.0013	0.1092	0.0056	0.2139	0.0159	0.2265	0.0093	0.2270	0.0048	0.2579	0.0203	0.2357	0.0044	0.2275	0.0001	0.2750	0.0220	0.2355	0.0045	0.2274	0.0006	0.2773	0.0222	0.2380	0.0032	0.2276	0.0007
s2	0.6492	0.0032	0.5732	0.2087	0.3809	0.0781	0.4729	0.0238	0.4958	0.0123	0.2999	0.1989	0.5400	0.0159	0.5198	0.0003	0.2685	0.2458	0.5383	0.0149	0.5176	0.0014	0.2644	0.2519	0.5570	0.0259	0.5240	0.0018
so	0.6357	0.0014	0.4167	0.2229	0.2926	0.0349	0.2948	0.0103	0.2995	0.0053	0.2403	0.0442	0.2964	0.0077	0.3044	0.0001	0.2200	0.0749	0.2964	0.0073	0.3039	0.0006	0.2174	0.0789	0.2968	0.0122	0.3052	0.0008
		MAX	1.7242	1.4751	0.9992	0.5018	0.9434	0.2213	0.9654	0.1148	0.7967	0.2540	0.9906	0.1123	0.9885	0.0030	0.7649	0.3416	0.9894	0.1150	0.9863	0.0135	0.7607	0.3564	1.0025	0.0968	0.9925	0.0165
		MAD	0.5244	0.4090	0.3390	0.1381	0.2918	0.0533	0.2773	0.0276	0.2833	0.0638	0.2611	0.0139	0.2623	0.0007	0.2661	0.0761	0.2618	0.0128	0.2637	0.0032	0.2641	0.0799	0.2537	0.0275	0.2597	0.0040
		RMS	0.6463	0.5368	0.3943	0.1760	0.3405	0.0696	0.3259	0.0361	0.3299	0.0835	0.3127	0.0212	0.3127	0.0009	0.3177	0.1054	0.3132	0.0202	0.3139	0.0042	0.3167	0.1105	0.3076	0.0360	0.3107	0.0052
		SD	0.3798	0.3496	0.2024	0.1096	0.1764	0.0450	0.1721	0.0234	0.1699	0.0541	0.1730	0.0161	0.1712	0.0006	0.1744	0.0733	0.1729	0.0158	0.1711	0.0027	0.1757	0.0767	0.1748	0.0234	0.1714	0.0034

Table S2. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. Reference values are computed as the mean of SD(T)/eN{Q,5}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	SD(T)/DZ – SD/TZ	SD(T)/TZ – SD/QZ	SD(T)/QZ – SD/5Z	SD(T)/e1{D,T}Z – SD/e1{T,Q}Z	SD(T)/e1{T,Q}Z – SD/e1{Q,5}Z	SD(T)/e2{D,T}Z – SD/e2{T,Q}Z	SD(T)/e2{T,Q}Z – SD/e2{Q,5}Z	SD(T)/e3{D,T}Z – SD/e3{T,Q}Z	SD(T)/e3{T,Q}Z – SD/e3{Q,5}Z
alcl	-0.0387	-0.1386	-0.1715	-0.1731	-0.1795	-0.1653	-0.1807	-0.1577	-0.1716
alf	0.3347	0.0648	-0.0478	0.0003	-0.1091	-0.0726	-0.1123	-0.0496	-0.1092
alh	0.0246	-0.0849	-0.1095	-0.0880	-0.1069	-0.0681	-0.1074	-0.0626	-0.1023
alh3	0.6219	-0.1275	-0.2393	-0.1907	-0.2778	-0.0840	-0.2771	-0.0920	-0.2658
bf	0.1667	0.0348	-0.0386	0.0070	-0.0504	-0.0308	-0.0545	-0.0174	-0.0280
bh	0.0388	-0.0401	-0.0553	-0.0480	-0.0580	-0.0331	-0.0586	-0.0283	-0.0539
bh3	0.6026	0.1224	-0.0048	-0.0447	-0.0662	0.0414	-0.0654	0.0318	-0.0522
c2h2	0.6688	0.0326	-0.1281	-0.1595	-0.1658	-0.0277	-0.1749	0.0287	-0.1163
c2h3f	0.4301	-0.0332	-0.1660	-0.1819	-0.2013	-0.1279	-0.2086	-0.0844	-0.1610
c2h4	0.5635	0.0455	-0.0870	-0.1143	-0.1173	-0.0065	-0.1249	0.0402	-0.0764
ccl2	-0.3293	-0.3840	-0.4893	-0.4078	-0.4910	-0.3821	-0.4904	-0.4025	-0.4796
cf2	-0.1934	-0.1847	-0.2067	-0.1520	-0.2148	-0.1408	-0.2154	-0.1383	-0.2102
ch2c	0.4265	-0.0113	-0.1245	-0.1485	-0.1504	-0.0581	-0.1566	-0.0196	-0.1163
ch2nh	0.1727	-0.0947	-0.1868	-0.1769	-0.2139	-0.1974	-0.2188	-0.1697	-0.1864
ch2–sing	0.0062	-0.0493	-0.0737	-0.0650	-0.0785	-0.0786	-0.0797	-0.0743	-0.0715
ch3f	0.1125	-0.0221	-0.0789	-0.0598	-0.0955	-0.0929	-0.0986	-0.0846	-0.0786
ch3nh2	0.1869	-0.0318	-0.1179	-0.0944	-0.1432	-0.1436	-0.1479	-0.1177	-0.1174
ch4	0.3001	0.0718	0.0035	0.0022	-0.0099	0.0277	-0.0138	0.0399	0.0114
c–hcoh	-0.0431	-0.1121	-0.1565	-0.1284	-0.1734	-0.1471	-0.1757	-0.1411	-0.1604
c–hono	-0.3742	-0.4036	-0.4252	-0.3716	-0.4409	-0.3547	-0.4405	-0.3556	-0.4449
cl2	-0.2065	-0.2326	-0.3432	-0.2759	-0.4169	-0.2612	-0.4152	-0.2807	-0.4083
clcn	0.1472	-0.3350	-0.4019	-0.3768	-0.4443	-0.2904	-0.4447	-0.2685	-0.4280
clf	-0.0648	-0.1646	-0.2338	-0.2268	-0.2921	-0.2312	-0.2889	-0.2452	-0.2931

System	$\frac{SD(T)/DZ}{-SD/TZ}$	$\frac{SD(T)/TZ}{-SD/QZ}$	$\frac{SD(T)/QZ}{-SD/5Z}$	$\frac{SD(T)/e1\{D,T\}Z}{-SD/e1\{T,Q\}Z}$	$\frac{SD(T)/e1\{T,Q\}Z}{-SD/e1\{Q,5\}Z}$	$\frac{SD(T)/e2\{D,T\}Z}{-SD/e2\{T,Q\}Z}$	$\frac{SD(T)/e2\{T,Q\}Z}{-SD/e2\{Q,5\}Z}$	$\frac{SD(T)/e3\{D,T\}Z}{-SD/e3\{T,Q\}Z}$	$\frac{SD(T)/e3\{T,Q\}Z}{-SD/e3\{Q,5\}Z}$
c-n2h2	-0.2480	-0.2678	-0.3087	-0.2693	-0.3301	-0.2766	-0.3318	-0.2730	-0.3195
co	0.1335	-0.0871	-0.1699	-0.1523	-0.1991	-0.2014	-0.2037	-0.1766	-0.1736
co2	0.1484	-0.1458	-0.2678	-0.2289	-0.3178	-0.3008	-0.3249	-0.2832	-0.2797
cs	-0.0192	-0.4246	-0.4736	-0.4838	-0.5046	-0.4145	-0.5049	-0.4012	-0.5137
cs2	0.0586	-0.6182	-0.6718	-0.5256	-0.7105	-0.4151	-0.7097	-0.4007	-0.7031
dioxirane	-0.2641	-0.3180	-0.3669	-0.3342	-0.3917	-0.3469	-0.3935	-0.3442	-0.3799
f2	-0.1102	-0.2239	-0.2449	-0.2519	-0.2605	-0.2379	-0.2598	-0.2426	-0.2599
f2co	-0.1202	-0.2094	-0.2924	-0.2237	-0.3283	-0.2520	-0.3326	-0.2402	-0.3038
fccf	0.5031	-0.1168	-0.2913	-0.3186	-0.3402	-0.2407	-0.3497	-0.1846	-0.2876
formic	0.0236	-0.1539	-0.2456	-0.1999	-0.2837	-0.2457	-0.2888	-0.2326	-0.2558
h2co	0.1254	-0.0897	-0.1684	-0.1543	-0.1947	-0.1922	-0.1991	-0.1689	-0.1709
h2o	-0.0366	-0.0429	-0.0634	-0.0398	-0.0713	-0.0442	-0.0723	-0.0410	-0.0657
h2s	0.0731	-0.1092	-0.1315	-0.0429	-0.1385	-0.0096	-0.1382	-0.0104	-0.1367
hccf	0.5762	-0.0403	-0.2063	-0.2410	-0.2518	-0.1401	-0.2612	-0.0842	-0.2009
hcl	0.0100	-0.0828	-0.0796	-0.0524	-0.0759	-0.0381	-0.0760	-0.0379	-0.0749
hcn	0.2941	-0.0983	-0.2226	-0.2214	-0.2585	-0.2176	-0.2653	-0.1787	-0.2209
hcno	0.1337	-0.2405	-0.3792	-0.3556	-0.4263	-0.4264	-0.4336	-0.3875	-0.3854
hf	-0.0201	-0.0301	-0.0388	-0.0326	-0.0430	-0.0353	-0.0434	-0.0345	-0.0409
hnc	0.2080	-0.0832	-0.1873	-0.1706	-0.2158	-0.2018	-0.2215	-0.1702	-0.1846
hnco	0.1994	-0.1431	-0.2821	-0.2410	-0.3301	-0.3241	-0.3378	-0.3042	-0.2877
hnnn	-0.2376	-0.3881	-0.4809	-0.4304	-0.5206	-0.4674	-0.5248	-0.4582	-0.4952
hno	-0.3075	-0.2867	-0.3095	-0.2784	-0.3257	-0.2747	-0.3254	-0.2746	-0.3215
hocl	-0.1786	-0.2437	-0.2907	-0.2877	-0.3289	-0.2886	-0.3276	-0.2997	-0.3269
hocn	0.1792	-0.1788	-0.3121	-0.2862	-0.3596	-0.3622	-0.3670	-0.3231	-0.3191
hof	-0.1281	-0.2304	-0.2360	-0.2088	-0.2419	-0.1946	-0.2414	-0.1967	-0.2429
honc	-0.0084	-0.2357	-0.3367	-0.3021	-0.3760	-0.3564	-0.3812	-0.3441	-0.3463
hooh	-0.2038	-0.2224	-0.2392	-0.1978	-0.2517	-0.1865	-0.2513	-0.1862	-0.2497

System	$\frac{SD(T)/DZ}{-SD/TZ}$	$\frac{SD(T)/TZ}{-SD/QZ}$	$\frac{SD(T)/QZ}{-SD/5Z}$	$\frac{SD(T)/e1\{D,T\}Z}{-SD/e1\{T,Q\}Z}$	$\frac{SD(T)/e1\{T,Q\}Z}{-SD/e1\{Q,5\}Z}$	$\frac{SD(T)/e2\{D,T\}Z}{-SD/e2\{T,Q\}Z}$	$\frac{SD(T)/e2\{T,Q\}Z}{-SD/e2\{Q,5\}Z}$	$\frac{SD(T)/e3\{D,T\}Z}{-SD/e3\{T,Q\}Z}$	$\frac{SD(T)/e3\{T,Q\}Z}{-SD/e3\{Q,5\}Z}$
ketene	0.5167	-0.0389	-0.2042	-0.2138	-0.2550	-0.1833	-0.2645	-0.1287	-0.2036
methanol	0.1231	-0.0365	-0.1052	-0.0806	-0.1285	-0.1203	-0.1323	-0.1101	-0.1077
n2	-0.0573	-0.2322	-0.3074	-0.2861	-0.3361	-0.3263	-0.3398	-0.3184	-0.3150
n2h4	-0.1281	-0.1611	-0.2153	-0.1617	-0.2346	-0.1749	-0.2369	-0.1678	-0.2202
n2o	-0.3203	-0.4033	-0.4765	-0.4240	-0.5179	-0.4459	-0.5213	-0.4393	-0.4977
nccn	0.4760	-0.2447	-0.4790	-0.4701	-0.5562	-0.4997	-0.5692	-0.4278	-0.4851
nh2cl	-0.2326	-0.2850	-0.3061	-0.2927	-0.3147	-0.2849	-0.3139	-0.2912	-0.3145
nh3	-0.0157	-0.0436	-0.0803	-0.0440	-0.0887	-0.0552	-0.0904	-0.0492	-0.0785
ocs	0.1599	-0.3312	-0.4126	-0.4235	-0.4638	-0.3336	-0.4644	-0.3081	-0.4445
oxirene	0.2930	-0.1816	-0.3132	-0.3417	-0.3429	-0.2560	-0.3492	-0.2171	-0.3061
p2	-0.4874	-0.9380	-0.9624	-0.8335	-0.9793	-0.7693	-0.9773	-0.7741	-0.9818
ph3	0.1607	-0.0667	-0.1118	0.0285	-0.1516	0.0779	-0.1490	0.0759	-0.1599
sih3f	0.7324	0.1605	0.0059	-0.0086	0.0302	0.1038	0.0288	0.0909	0.0546
sih4	0.7226	-0.0551	-0.0969	0.0482	-0.0301	0.1632	-0.0323	0.1615	-0.0139
sio	0.2884	-0.1080	-0.2504	-0.2225	-0.3346	-0.3180	-0.3370	-0.2957	-0.2952
so2	-0.1700	-0.5468	-0.5962	-0.5142	-0.6132	-0.4558	-0.6126	-0.4525	-0.6090
t-hcoh	-0.0205	-0.1058	-0.1528	-0.1280	-0.1679	-0.1500	-0.1703	-0.1438	-0.1544
t-hono	-0.3882	-0.4146	-0.4376	-0.3869	-0.4547	-0.3713	-0.4542	-0.3726	-0.4584
t-n2h2	-0.2284	-0.2608	-0.3052	-0.2668	-0.3236	-0.2766	-0.3252	-0.2728	-0.3126
cch	0.5916	-0.0094	-0.1540	-0.1633	-0.1850	-0.0408	-0.1929	0.0095	-0.1414
cf	-0.0715	-0.0831	-0.1048	-0.0831	-0.1084	-0.0879	-0.1092	-0.0853	-0.1030
ch	-0.0298	-0.0409	-0.0506	-0.0436	-0.0521	-0.0466	-0.0524	-0.0456	-0.0498
ch2ch	0.5650	0.0486	-0.0784	-0.0916	-0.1056	0.0148	-0.1128	0.0600	-0.0667
ch2nh2	0.2635	-0.0151	-0.1081	-0.1008	-0.1247	-0.0894	-0.1294	-0.0605	-0.0979
ch3	0.3012	0.0765	0.0164	-0.0053	0.0077	0.0451	0.0044	0.0362	0.0260
ch3nh	0.1670	-0.0322	-0.1072	-0.0909	-0.1289	-0.1235	-0.1329	-0.1010	-0.1066
clo	-0.2192	-0.2566	-0.3178	-0.2930	-0.3713	-0.2870	-0.3680	-0.2999	-0.3825

System	$\frac{SD(T)/DZ}{-SD/TZ}$	$\frac{SD(T)/TZ}{-SD/QZ}$	$\frac{SD(T)/QZ}{-SD/5Z}$	$\frac{SD(T)/e1\{D,T\}Z}{-SD/e1\{T,Q\}Z}$	$\frac{SD(T)/e1\{T,Q\}Z}{-SD/e1\{Q,5\}Z}$	$\frac{SD(T)/e2\{D,T\}Z}{-SD/e2\{T,Q\}Z}$	$\frac{SD(T)/e2\{T,Q\}Z}{-SD/e2\{Q,5\}Z}$	$\frac{SD(T)/e3\{D,T\}Z}{-SD/e3\{T,Q\}Z}$	$\frac{SD(T)/e3\{T,Q\}Z}{-SD/e3\{Q,5\}Z}$
cn	0.0517	-0.1238	-0.1690	-0.1545	-0.1687	-0.2085	-0.1763	-0.1869	-0.1772
h2cn	0.2073	-0.0879	-0.1803	-0.1817	-0.2063	-0.1726	-0.2112	-0.1442	-0.1788
hcnh	0.2028	-0.0905	-0.1852	-0.1832	-0.2076	-0.1740	-0.2125	-0.1454	-0.1800
hco	0.1608	-0.0775	-0.1579	-0.1515	-0.1811	-0.1636	-0.1854	-0.1394	-0.1572
hoo	-0.1625	-0.2137	-0.2215	-0.1989	-0.2279	-0.1889	-0.2276	-0.1905	-0.2294
hs	0.0241	-0.0565	-0.0709	-0.0312	-0.0692	-0.0161	-0.0692	-0.0177	-0.0676
n2h	-0.1368	-0.2351	-0.2903	-0.2643	-0.3106	-0.2876	-0.3130	-0.2825	-0.2961
nh2	-0.0645	-0.0511	-0.0712	-0.0405	-0.0767	-0.0412	-0.0775	-0.0380	-0.0716
no	-0.2097	-0.2407	-0.2715	-0.2504	-0.2889	-0.2575	-0.2900	-0.2562	-0.2814
no2	-0.4137	-0.3998	-0.4313	-0.3958	-0.4534	-0.3925	-0.4530	-0.3933	-0.4529
oh	-0.0449	-0.0348	-0.0433	-0.0290	-0.0465	-0.0282	-0.0468	-0.0271	-0.0446
sif	0.0732	-0.0161	-0.0778	-0.0324	-0.1148	-0.0595	-0.1157	-0.0489	-0.0998
sih	0.0166	-0.0719	-0.0760	-0.0409	-0.0806	-0.0265	-0.0801	-0.0263	-0.0813
ssh	-0.1262	-0.2454	-0.3700	-0.2208	-0.4283	-0.1740	-0.4269	-0.1933	-0.4170
ch2-trip	0.3000	0.0920	0.0265	-0.0242	-0.0127	0.0213	-0.0123	0.0142	-0.0037
nh	-0.0424	-0.0377	-0.0452	-0.0271	-0.0470	-0.0238	-0.0471	-0.0228	-0.0456
o2	-0.2082	-0.2105	-0.2177	-0.2154	-0.2231	-0.2135	-0.2229	-0.2158	-0.2244
s2	-0.1722	-0.3947	-0.4720	-0.3411	-0.5039	-0.2926	-0.5026	-0.3051	-0.4981
so	-0.0696	-0.2598	-0.2892	-0.2522	-0.2967	-0.2214	-0.2967	-0.2179	-0.2930
MAX	0.4760	-0.4416	-0.7441	-0.7366	-0.8762	-0.6479	-0.8713	-0.6461	-0.8958
MAD	0.0700	-0.1536	-0.2240	-0.1972	-0.2484	-0.1857	-0.2509	-0.1739	-0.2322
RMS	0.1425	-0.1645	-0.2563	-0.2292	-0.2915	-0.2078	-0.2936	-0.1972	-0.2747
SD	0.1472	-0.0668	-0.1270	-0.1189	-0.1550	-0.0996	-0.1553	-0.0981	-0.1480

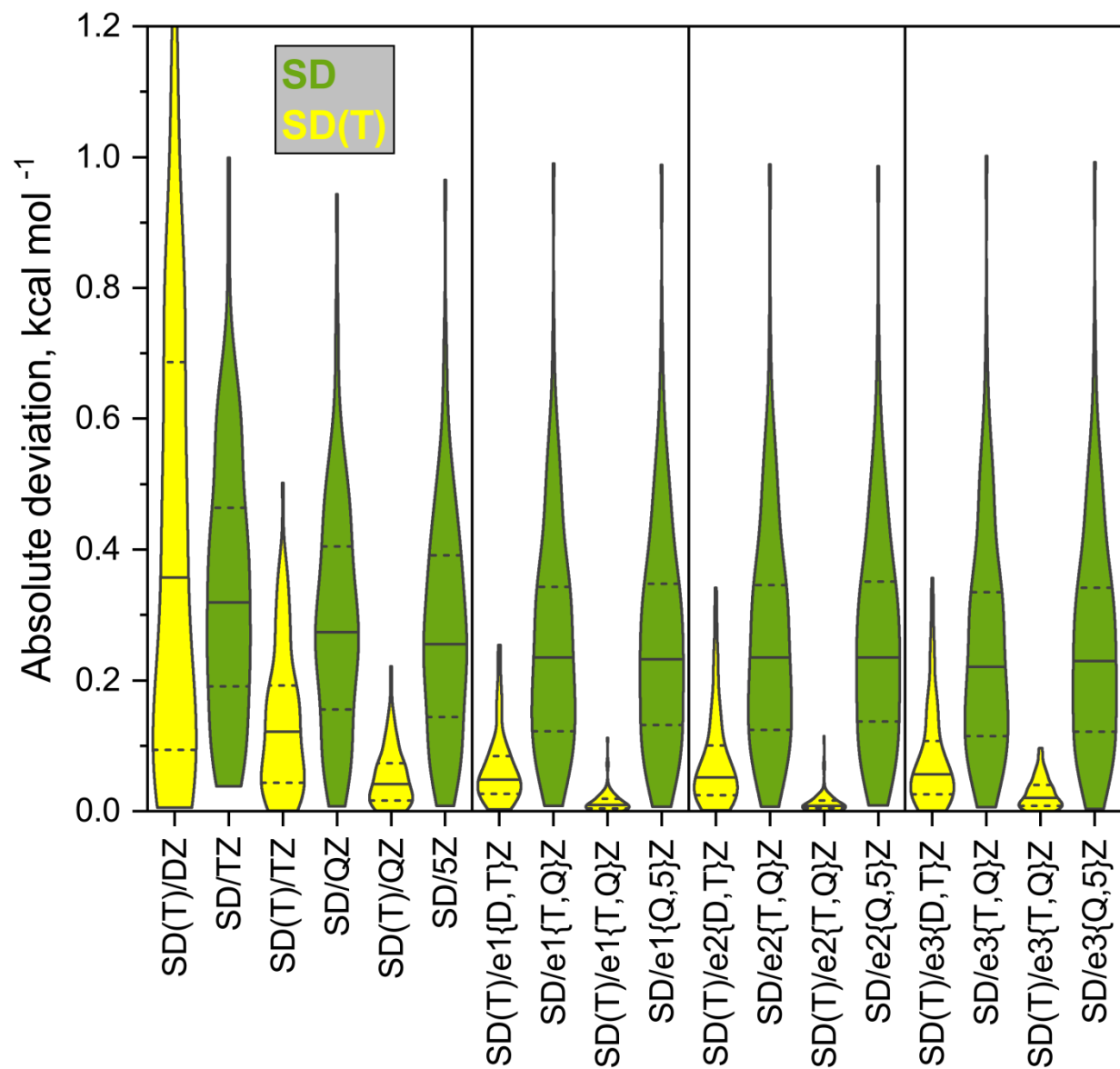


Figure S1. Violin plots of the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SD(T)/eN{Q,5}Z (N = 1 – 3) values. The median (solid), 25th, and 75th percentiles (dash) are shown. The highest point of a plot represents the maximum deviation.

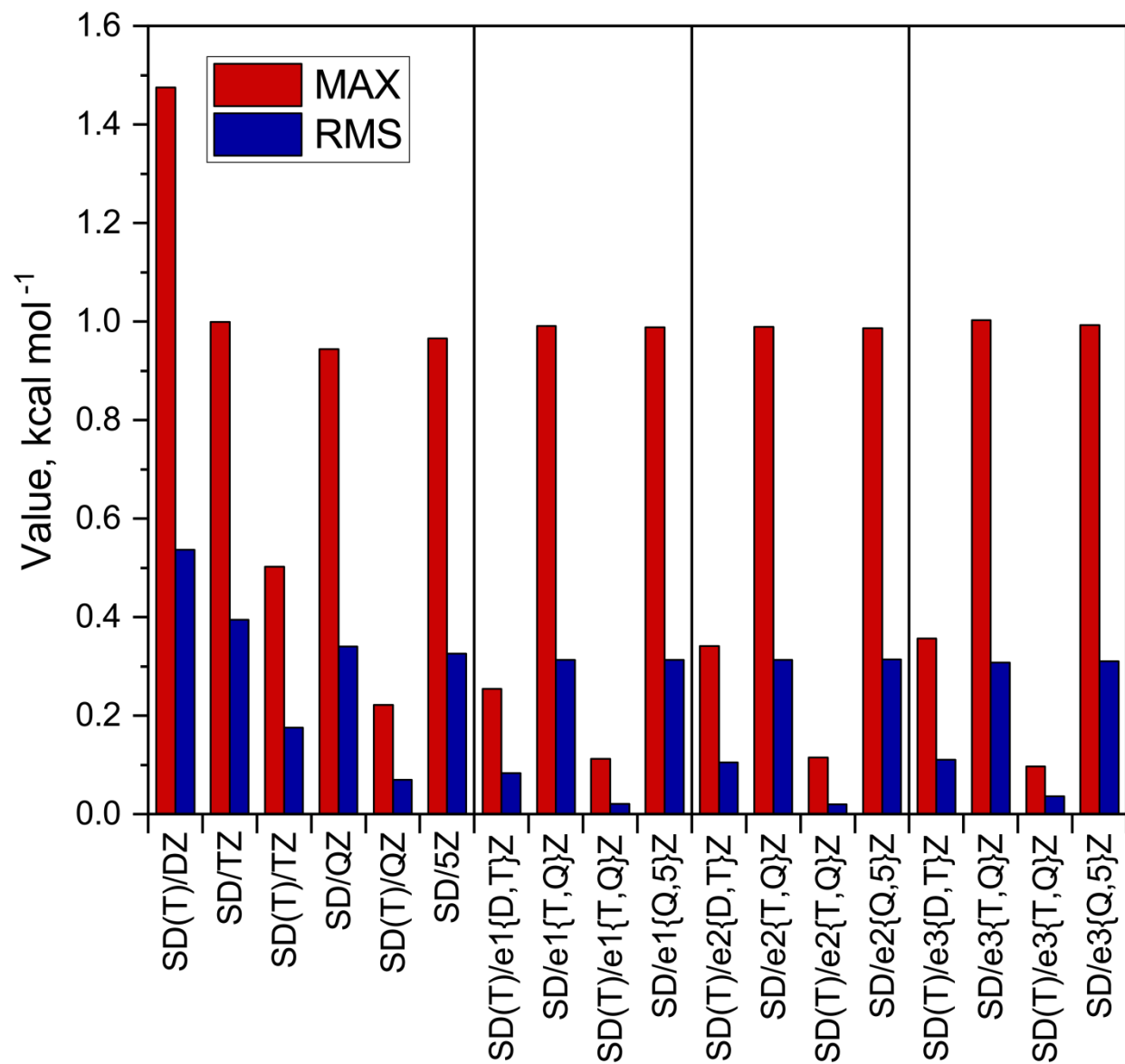


Figure S2. Maximum (MAX) and root mean square (RMS) values for the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SD(T)/eN{Q,5}Z (N = 1 – 3) values.

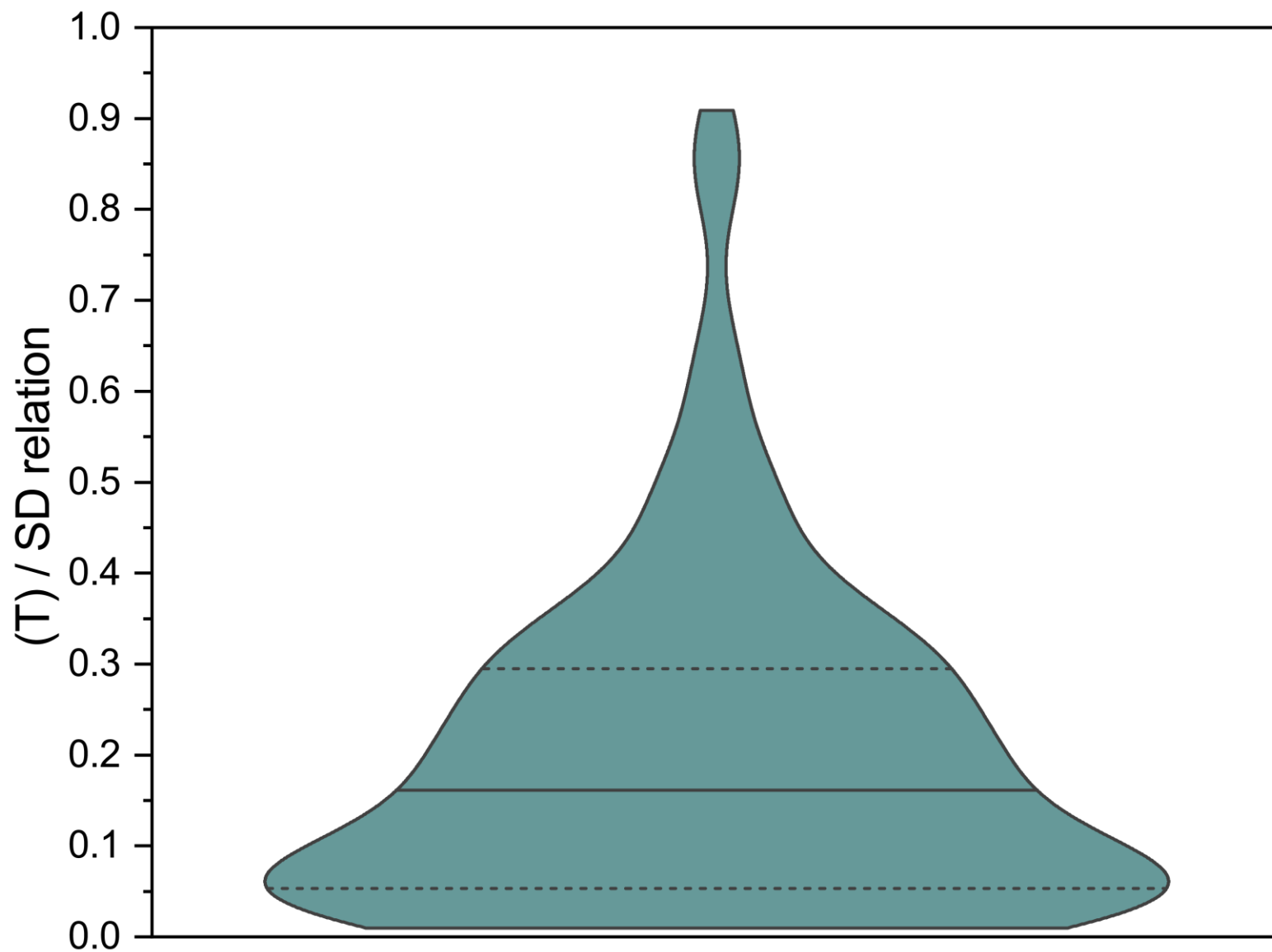


Figure S3. The relations between computational times for perturbative triples and iterative singles and doubles. The times for the FC and CV $\text{SD}(T)/nZ$ ($n = D, T, Q, 5$) computations were combined and used for visualization. Times lower than 1 min were excluded. The median (solid), 25th, and 75th percentiles (dash) are shown.

Batch #2

Table S3. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values. The range of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values (RANGE, RMS = 0.0114 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SD(T)/DZ	SDT/DZ	SDT(Q)/DZ	SD(T)/TZ	SDT/TZ	SDT(Q)/TZ	SD(T)/QZ	SDT/QZ	SDT(Q)/QZ	SD(T)/e1{D,T}Z	SDT/e1{D,T}Z	SDT(Q)/e1{D,T}Z	SD(T)/e1{T,Q}Z	SDT/e1{T,Q}Z	SDT(Q)/e1{T,Q}Z	SD(T)/e2{D,T}Z	SDT/e2{D,T}Z	SDT(Q)/e2{D,T}Z	SD(T)/e2{T,Q}Z	SDT/e2{T,Q}Z	SDT(Q)/e2{T,Q}Z	SD(T)/e3{D,T}Z	SDT/e3{D,T}Z	SDT(Q)/e3{D,T}Z	SD(T)/e3{T,Q}Z	SDT/e3{T,Q}Z	SDT(Q)/e3{T,Q}Z
alh	-0.0735	0.0046	0.1838	0.1709	0.1756	0.0602	0.0326	0.0446	0.0353	0.0055	0.0198	0.0081	0.0257	0.0105	0.0172	0.0142	0.0016	0.0121	0.0470	0.0318	0.0176	0.0143	0.0013	0.0147	0.0512	0.0347	0.0126	0.0192	0.0029
bf	0.8417	0.0197	0.4268	0.4193	0.4140	0.2051	0.1886	0.1797	0.1076	0.0883	0.0792	0.1117	0.0915	0.0811	0.0365	0.0151	0.0058	0.0755	0.0546	0.0442	0.0383	0.0162	0.0069	0.0708	0.0489	0.0378	0.0185	0.0034	0.0127
bh	0.2320	0.0037	0.1399	0.1352	0.1365	0.0470	0.0340	0.0361	0.0283	0.0137	0.0160	0.0079	0.0086	0.0061	0.0146	0.0011	0.0013	0.0073	0.0244	0.0219	0.0150	0.0011	0.0012	0.0093	0.0273	0.0247	0.0112	0.0048	0.0025
bh3	1.1740	0.0202	0.6955	0.6943	0.6990	0.1789	0.1758	0.1825	0.0777	0.0730	0.0804	0.0386	0.0425	0.0350	0.0038	0.0020	0.0058	0.1229	0.1270	0.1195	0.0056	0.0006	0.0072	0.1340	0.1382	0.1304	0.0148	0.0210	0.0130
ch2-sing	0.5089	0.0065	0.1770	0.1633	0.1626	0.0964	0.0631	0.0628	0.0654	0.0283	0.0278	0.0625	0.0209	0.0207	0.0427	0.0030	0.0022	0.0494	0.0062	0.0061	0.0433	0.0027	0.0020	0.0477	0.0024	0.0023	0.0370	0.0034	0.0042
co	1.2045	0.0224	0.5629	0.5594	0.5453	0.2525	0.2252	0.2080	0.1420	0.1098	0.0917	0.1218	0.0846	0.0660	0.0615	0.0255	0.0068	0.0711	0.0321	0.0135	0.0634	0.0263	0.0078	0.0644	0.0229	0.0038	0.0411	0.0042	0.0146
f2	0.0599	0.0026	0.0501	0.0566	0.0661	0.0318	0.0037	0.0105	0.0440	0.0027	0.0043	0.0664	0.0185	0.0130	0.0529	0.0075	0.0001	0.0798	0.0297	0.0241	0.0526	0.0059	0.0014	0.0815	0.0283	0.0233	0.0551	0.0087	0.0012
h2o	0.4947	0.0054	0.0840	0.0844	0.0808	0.0593	0.0538	0.0490	0.0338	0.0273	0.0216	0.0490	0.0410	0.0356	0.0152	0.0079	0.0016	0.0450	0.0365	0.0311	0.0156	0.0082	0.0019	0.0444	0.0353	0.0298	0.0105	0.0030	0.0035
h2s	0.4461	0.0036	0.1797	0.1916	0.1907	0.0216	0.0239	0.0232	0.0055	0.0112	0.0100	0.1064	0.1146	0.1132	0.0062	0.0020	0.0004	0.1393	0.1486	0.1472	0.0059	0.0031	0.0016	0.1436	0.1544	0.1527	0.0092	0.0003	0.0020
hcl	0.2626	0.0008	0.0806	0.0907	0.0881	0.0058	0.0009	0.0036	0.0012	0.0037	0.0015	0.0422	0.0369	0.0422	0.0021	0.0057	0.0000	0.0563	0.0513	0.0566	0.0020	0.0052	0.0004	0.0582	0.0535	0.0592	0.0030	0.0062	0.0004
hf	0.2374	0.0024	0.0381	0.0390	0.0365	0.0226	0.0235	0.0189	0.0124	0.0139	0.0083	0.0160	0.0170	0.0115	0.0049	0.0069	0.0005	0.0135	0.0145	0.0089	0.0051	0.0072	0.0010	0.0132	0.0141	0.0082	0.0030	0.0051	0.0015
n2	1.1569	0.0191	0.4817	0.4775	0.4623	0.2428	0.1979	0.1854	0.1479	0.0945	0.0820	0.1423	0.0802	0.0689	0.0787	0.0191	0.0064	0.1033	0.0380	0.0268	0.0804	0.0189	0.0062	0.0982	0.0285	0.0178	0.0611	0.0000	0.0127
nh3	0.8124	0.0093	0.1696	0.1681	0.1652	0.1050	0.0899	0.0884	0.0591	0.0408	0.0390	0.0778	0.0569	0.0560	0.0256	0.0050	0.0030	0.0673	0.0453	0.0445	0.0264	0.0051	0.0031	0.0659	0.0424	0.0419	0.0171	0.0040	0.0061
cf	0.4550	0.0054	0.1053	0.1023	0.0942	0.0780	0.0644	0.0512	0.0526	0.0368	0.0226	0.0665	0.0485	0.0331	0.0340	0.0167	0.0017	0.0621	0.0432	0.0278	0.0344	0.0166	0.0018	0.0615	0.0415	0.0251	0.0293	0.0116	0.0035
ch	0.2006	0.0023	0.0517	0.0481	0.0482	0.0339	0.0222	0.0227	0.0229	0.0097	0.0100	0.0264	0.0113	0.0119	0.0149	0.0007	0.0008	0.0235	0.0078	0.0084	0.0151	0.0005	0.0007	0.0231	0.0065	0.0072	0.0129	0.0016	0.0015
ch3	1.1435	0.0159	0.4484	0.4472	0.4483	0.1483	0.1411	0.1447	0.0686	0.0597	0.0638	0.0219	0.0123	0.0169	0.0104	0.0002	0.0047	0.0271	0.0372	0.0325	0.0118	0.0012	0.0056	0.0335	0.0443	0.0391	0.0043	0.0148	0.0103
cn	1.3950	0.0288	0.6595	0.6382	0.6116	0.3441	0.2922	0.2650	0.1947	0.1399	0.1168	0.2113	0.1465	0.1190	0.0857	0.0288	0.0086	0.1598	0.0927	0.0652	0.0883	0.0308	0.0101	0.1530	0.0827	0.0551	0.0581	0.0007	0.0187
hs	0.2242	0.0024	0.0734	0.0802	0.0811	0.0168	0.0187	0.0177	0.0053	0.0087	0.0077	0.0548	0.0604	0.0593	0.0032	0.0014	0.0004	0.0695	0.0758	0.0747	0.0030	0.0019	0.0010	0.0714	0.0787	0.0775	0.0053	0.0005	0.0014
nh2	0.4433	0.0049	0.0602	0.0595	0.0578	0.0576	0.0475	0.0466	0.0339	0.0220	0.0206	0.0565	0.0425	0.0419	0.0165	0.0033	0.0016	0.0561	0.0413	0.0407	0.0170	0.0033	0.0016	0.0561	0.0403	0.0398	0.0121	0.0014	0.0032

System	REFERENCE	RANGE	SD(T)/DZ	SDT/DZ	SDT(Q)/DZ	SD(T)/TZ	SDT/TZ	SDT(Q)/TZ	SD(T)/QZ	SDT/QZ	SDT(Q)/QZ	SD(T)/e1{D,T}Z	SDT/e1{D,T}Z	SDT(Q)/e1{D,T}Z	SD(T)/e1{T,Q}Z	SDT/e1{T,Q}Z	SDT(Q)/e1{T,Q}Z	SD(T)/e2{D,T}Z	SDT/e2{D,T}Z	SDT(Q)/e2{D,T}Z	SD(T)/e2{T,Q}Z	SDT/e2{T,Q}Z	SDT(Q)/e2{T,Q}Z	SD(T)/e3{D,T}Z	SDT/e3{D,T}Z	SDT(Q)/e3{D,T}Z	SD(T)/e3{T,Q}Z	SDT/e3{T,Q}Z	SDT(Q)/e3{T,Q}Z
no	0.6987	0.0080	0.1742	0.1709	0.1547	0.1324	0.0951	0.0782	0.0968	0.0524	0.0347	0.1148	0.0631	0.0460	0.0708	0.0213	0.0030	0.1080	0.0537	0.0366	0.0714	0.0203	0.0021	0.1071	0.0492	0.0319	0.0642	0.0134	0.0051
oh	0.2108	0.0021	0.0184	0.0188	0.0171	0.0236	0.0214	0.0188	0.0140	0.0115	0.0083	0.0258	0.0225	0.0195	0.0070	0.0044	0.0006	0.0266	0.0231	0.0202	0.0072	0.0045	0.0008	0.0267	0.0229	0.0199	0.0053	0.0025	0.0014
sih	0.0464	0.0006	0.1029	0.1000	0.1042	0.0158	0.0063	0.0024	0.0146	0.0093	0.0012	0.0209	0.0511	0.0404	0.0138	0.0114	0.0003	0.0351	0.0668	0.0561	0.0138	0.0118	0.0003	0.0370	0.0708	0.0592	0.0136	0.0119	0.0000
ch2-trip	0.8604	0.0130	0.3868	0.3870	0.3890	0.1152	0.1132	0.1168	0.0503	0.0475	0.0514	0.0009	0.0020	0.0022	0.0029	0.0005	0.0037	0.0435	0.0465	0.0423	0.0041	0.0005	0.0046	0.0493	0.0525	0.0480	0.0090	0.0126	0.0084
nh	0.1739	0.0016	0.0001	0.0000	0.0006	0.0206	0.0159	0.0155	0.0131	0.0076	0.0069	0.0293	0.0225	0.0223	0.0077	0.0015	0.0005	0.0326	0.0255	0.0253	0.0078	0.0015	0.0005	0.0331	0.0255	0.0253	0.0063	0.0000	0.0011
o2	0.4223	0.0025	0.0562	0.0551	0.0432	0.0666	0.0334	0.0252	0.0599	0.0195	0.0114	0.0709	0.0243	0.0177	0.0550	0.0093	0.0014	0.0726	0.0235	0.0169	0.0551	0.0077	0.0002	0.0728	0.0203	0.0143	0.0538	0.0067	0.0012
		MAX	0.6955	0.6943	0.6990	0.3441	0.2922	0.2650	0.1947	0.1399	0.1168	0.2113	0.1465	0.1190	0.0857	0.0288	0.0086	0.1598	0.1486	0.1472	0.0883	0.0308	0.0101	0.1530	0.1544	0.1527	0.0642	0.0210	0.0187
		MAD	0.2163	0.2143	0.2109	0.0953	0.0794	0.0759	0.0555	0.0375	0.0335	0.0620	0.0458	0.0396	0.0274	0.0086	0.0025	0.0624	0.0477	0.0409	0.0280	0.0086	0.0029	0.0628	0.0473	0.0403	0.0227	0.0065	0.0053
		RMS	0.2987	0.2953	0.2909	0.1290	0.1115	0.1057	0.0737	0.0524	0.0466	0.0790	0.0575	0.0501	0.0373	0.0118	0.0035	0.0736	0.0580	0.0522	0.0381	0.0120	0.0040	0.0737	0.0590	0.0535	0.0304	0.0088	0.0074
		SD	0.2103	0.2074	0.2044	0.0888	0.0800	0.0751	0.0496	0.0374	0.0331	0.0499	0.0355	0.0313	0.0259	0.0083	0.0025	0.0398	0.0338	0.0331	0.0263	0.0086	0.0028	0.0394	0.0360	0.0358	0.0206	0.0061	0.0053

Table S4. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. Reference values are computed as the mean of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	$\frac{\text{SDT/DZ}}{\text{SD(T)/TZ}}$	$\frac{\text{SDT(Q)/DZ}}{\text{SD(T)/TZ}}$	$\frac{\text{SDT/TZ}}{\text{SD(T)/QZ}}$	$\frac{\text{SDT(Q)/TZ}}{\text{SD(T)/QZ}}$	$\frac{\text{SDT/e1{D,T}Z}}{\text{SD(T)/e1{T,Q}Z}}$	$\frac{\text{SDT(Q)/e1{D,T}Z}}{\text{SD(T)/e1{T,Q}Z}}$	$\frac{\text{SDT/e2{D,T}Z}}{\text{SD(T)/e2{T,Q}Z}}$	$\frac{\text{SDT(Q)/e2{D,T}Z}}{\text{SD(T)/e2{T,Q}Z}}$	$\frac{\text{SDT/e3{D,T}Z}}{\text{SD(T)/e3{T,Q}Z}}$	$\frac{\text{SDT(Q)/e3{D,T}Z}}{\text{SD(T)/e3{T,Q}Z}}$
alh	0.1107	0.1430	-0.0028	0.0391	0.0085	-0.0037	0.0293	0.0175	0.0386	0.0155
bf	0.2142	0.2253	0.0810	0.0914	0.0550	0.0660	0.0164	0.0280	0.0304	0.0344
bh	0.0882	0.1025	0.0058	0.0224	-0.0061	0.0050	0.0094	0.0208	0.0161	0.0198
bh3	0.5154	0.5232	0.0981	0.1095	0.0387	0.0330	0.1213	0.1189	0.1234	0.1094
ch2-sing	0.0668	0.0995	-0.0023	0.0344	-0.0219	0.0178	-0.0371	0.0034	-0.0347	-0.0011
co	0.3069	0.3200	0.0832	0.0982	0.0231	0.0405	-0.0314	-0.0128	-0.0182	-0.0005
f2	0.0247	0.0624	-0.0402	0.0077	-0.0344	0.0055	-0.0230	0.0182	-0.0268	0.0146
h2o	0.0250	0.0269	0.0200	0.0217	0.0258	0.0277	0.0208	0.0230	0.0248	0.0267
h2s	0.1700	0.1668	0.0184	0.0119	0.1084	0.1112	0.1426	0.1441	0.1452	0.1524
hcl	0.0849	0.0872	-0.0003	0.0000	0.0348	0.0366	0.0493	0.0514	0.0506	0.0530
hf	0.0164	0.0130	0.0112	0.0050	0.0121	0.0045	0.0094	0.0017	0.0111	0.0031
n2	0.2346	0.2644	0.0500	0.0909	0.0015	0.0498	-0.0423	0.0079	-0.0326	0.0177
nh3	0.0631	0.0753	0.0308	0.0476	0.0313	0.0510	0.0189	0.0393	0.0254	0.0378
cf	0.0243	0.0298	0.0118	0.0144	0.0145	0.0164	0.0087	0.0112	0.0122	0.0135
ch	0.0142	0.0260	-0.0008	0.0130	-0.0037	0.0113	-0.0074	0.0079	-0.0064	0.0056
ch3	0.2989	0.3072	0.0726	0.0851	0.0018	0.0167	0.0254	0.0313	0.0400	0.0243
cn	0.2941	0.3194	0.0975	0.1251	0.0609	0.0903	0.0044	0.0344	0.0246	0.0544
hs	0.0634	0.0623	0.0135	0.0090	0.0572	0.0579	0.0728	0.0728	0.0734	0.0770
nh2	0.0019	0.0103	0.0137	0.0246	0.0260	0.0385	0.0244	0.0374	0.0281	0.0384
no	0.0385	0.0596	-0.0017	0.0258	-0.0076	0.0247	-0.0177	0.0163	-0.0150	0.0185
oh	-0.0048	-0.0042	0.0073	0.0073	0.0154	0.0152	0.0159	0.0157	0.0177	0.0173
sih	0.0842	0.0978	-0.0083	-0.0068	0.0373	0.0290	0.0530	0.0443	0.0572	0.0472

System	$\frac{SDT/DZ}{-SD(T)/TZ}$	$\frac{SDT(Q)/DZ}{-SDT/TZ}$	$\frac{SDT/TZ}{-SD(T)/QZ}$	$\frac{SDT(Q)/TZ}{-SDT/QZ}$	$\frac{SDT/e1\{D,T\}Z}{-SD(T)/e1\{T,Q\}Z}$	$\frac{SDT(Q)/e1\{D,T\}Z}{-SDT/e1\{T,Q\}Z}$	$\frac{SDT/e2\{D,T\}Z}{-SD(T)/e2\{T,Q\}Z}$	$\frac{SDT(Q)/e2\{D,T\}Z}{-SDT/e2\{T,Q\}Z}$	$\frac{SDT/e3\{D,T\}Z}{-SD(T)/e3\{T,Q\}Z}$	$\frac{SDT(Q)/e3\{D,T\}Z}{-SDT/e3\{T,Q\}Z}$
ch2-trip	0.2718	0.2757	0.0630	0.0693	-0.0009	0.0018	0.0424	0.0418	0.0435	0.0354
nh	-0.0206	-0.0153	0.0027	0.0079	0.0149	0.0208	0.0177	0.0238	0.0192	0.0252
o2	-0.0114	0.0098	-0.0265	0.0058	-0.0308	0.0084	-0.0317	0.0092	-0.0335	0.0076
MAX	0.3502	0.4068	0.0975	0.1251	0.0609	0.0903	0.0602	0.1164	0.0902	0.1317
MAD	0.1190	0.1315	0.0239	0.0384	0.0185	0.0310	0.0197	0.0323	0.0246	0.0339
RMS	0.1663	0.1793	0.0378	0.0533	0.0202	0.0382	0.0199	0.0402	0.0286	0.0447
SD	0.1186	0.1245	0.0304	0.0377	0.0096	0.0230	0.0074	0.0245	0.0154	0.0298

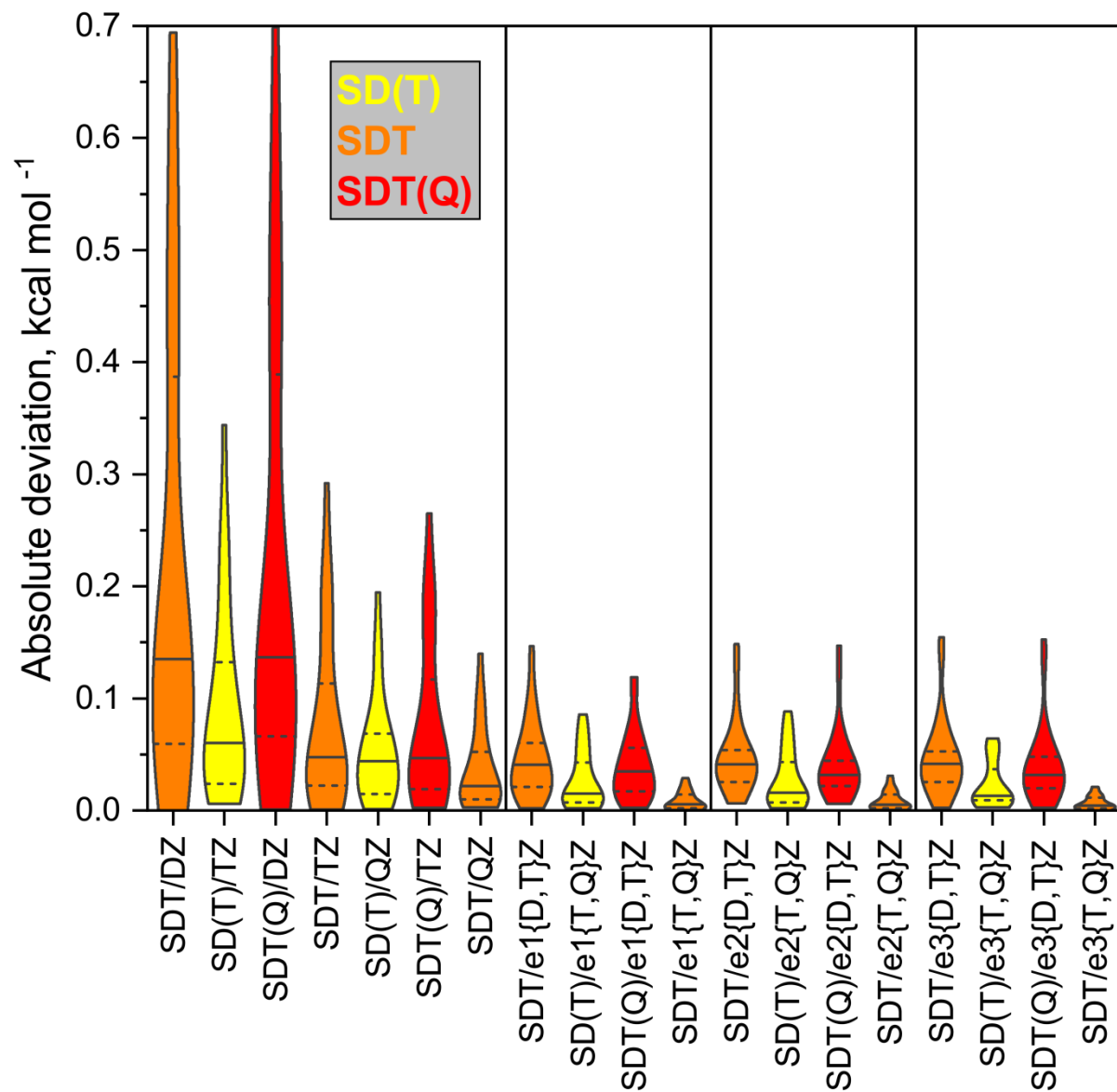


Figure S4. Violin plots of the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of $\text{SDT(Q)}/eN\{\text{T,Q}\}Z$ ($N = 1 - 3$) values. The median (solid), 25th, and 75th percentiles (dash) are shown. The highest point of a plot represents the maximum deviation.

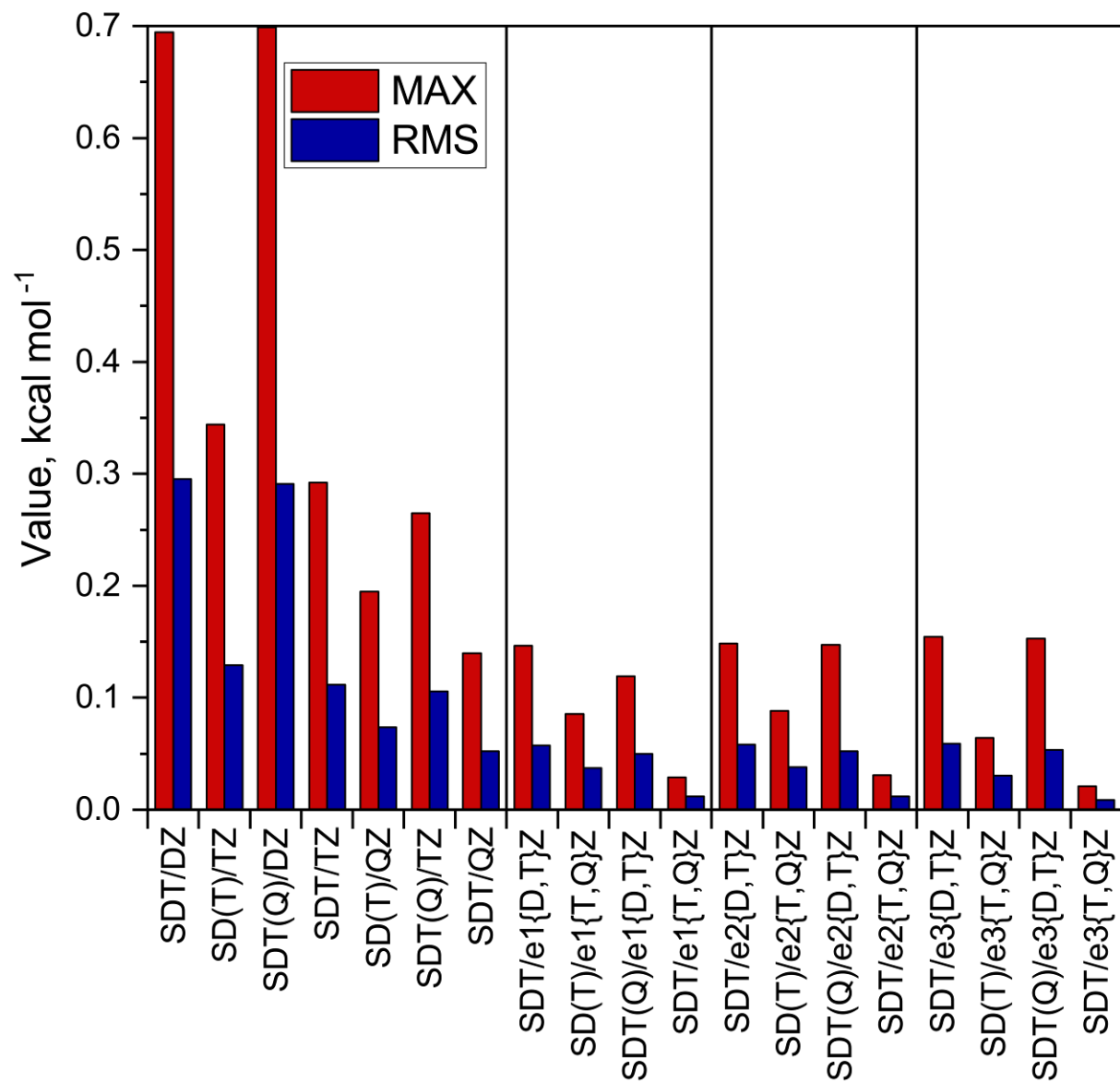


Figure S5. Maximum (MAX) and root mean square (RMS) values for the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of $\text{SDT(Q)/eN}\{T,Q\}Z$ ($N = 1 - 3$) values.

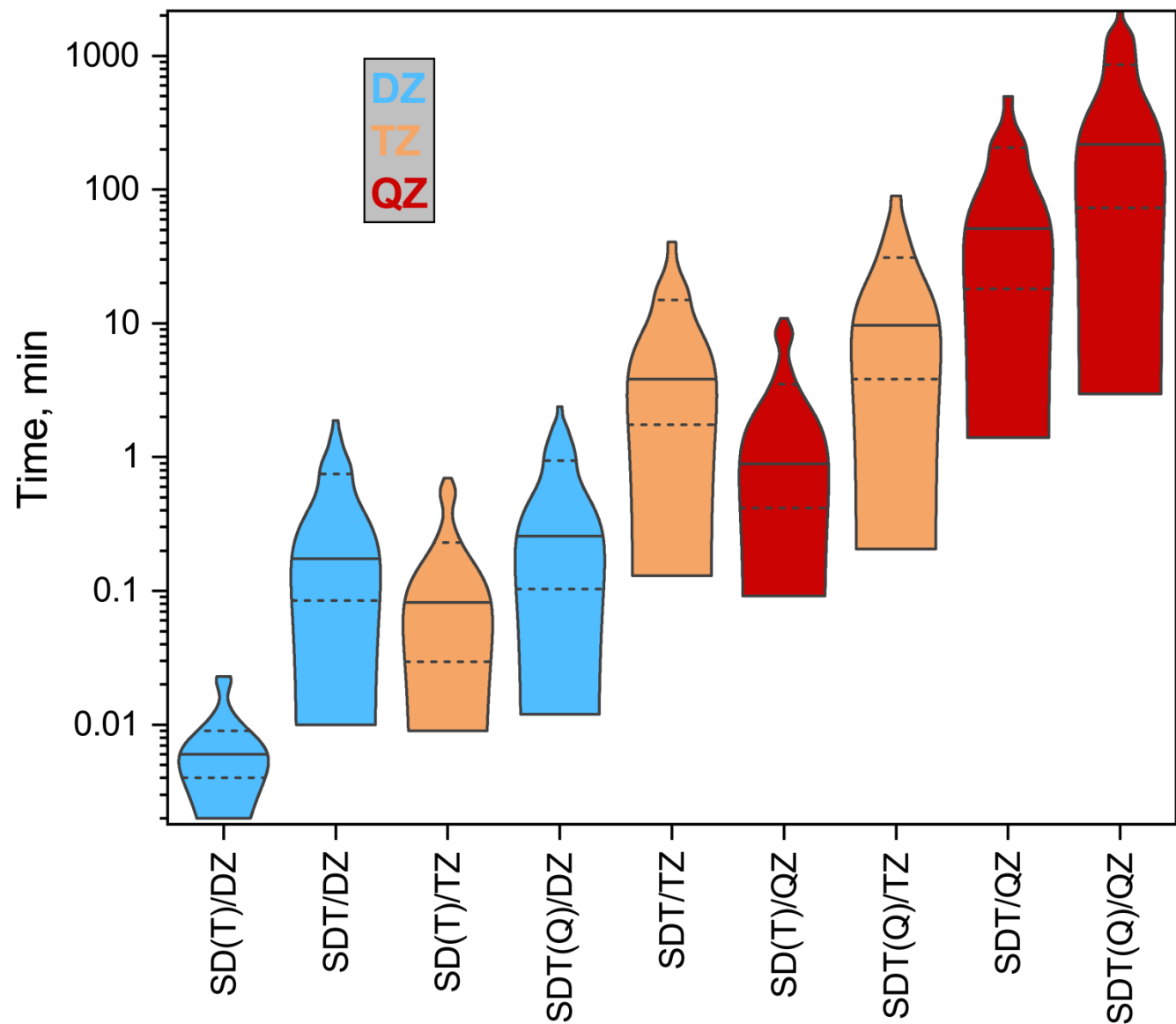


Figure S6. Computational times for different levels of theory. The times for the FC and CV calculations were combined and used for the visualization. The data for the SD(T) method were obtained using the optimized CCSD(T) program “ccsd” for systems for which SDT(Q) computations were performed. The median (solid), 25th, and 75th percentiles (dash) are shown.

Batches #3 and #4

Table S5. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SDTQ(P)/eN{D,T}Z (N = 1 – 3) values. The range of SDTQ(P)/eN{D,T}Z (N = 1 – 3) values (RANGE, RMS = 0.0389 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SDT(Q)/DZ	SDTQ/DZ	SDTQ(P)/DZ	SDT(Q)/TZ	SDTQ/TZ	SDTQ(P)/TZ	SDT(Q)/e1{D,T}Z	SDTQ/e1{D,T}Z	SDTQ(P)/e1{D,T}Z	SDT(Q)/e2{D,T}Z	SDTQ/e2{D,T}Z	SDTQ(P)/e2{D,T}Z	SDT(Q)/e3{D,T}Z	SDTQ/e3{D,T}Z	SDTQ(P)/e3{D,T}Z
bh3	1.26786	0.09526	0.79286	0.79310	0.79316	0.27634	0.27679	0.27718	0.05886	0.05940	0.05992	0.02563	0.02497	0.02459	0.03650	0.03593	0.03534
ch2–sing	0.49873	0.01836	0.15241	0.15241	0.15238	0.05261	0.05258	0.05294	0.01058	0.01054	0.01107	0.00407	0.00413	0.00377	0.00784	0.00789	0.00729
h2o	0.46196	0.00582	0.04805	0.04841	0.04812	0.01629	0.01711	0.01659	0.00292	0.00394	0.00331	0.00155	0.00027	0.00080	0.00294	0.00184	0.00251
hf	0.22761	0.00325	0.02671	0.02702	0.02687	0.00908	0.00961	0.00927	0.00166	0.00228	0.00186	0.00088	0.00013	0.00047	0.00160	0.00093	0.00139
ch	0.19136	0.00468	0.03899	0.03882	0.03880	0.01345	0.01327	0.01344	0.00270	0.00251	0.00276	0.00083	0.00102	0.00084	0.00202	0.00221	0.00192
ch3	1.16100	0.05596	0.46589	0.46591	0.46585	0.16229	0.16254	0.16275	0.03446	0.03481	0.03514	0.01500	0.01452	0.01431	0.02159	0.02120	0.02082
nh2	0.40206	0.00201	0.01660	0.01664	0.01646	0.00539	0.00571	0.00559	0.00067	0.00110	0.00101	0.00047	0.00012	0.00000	0.00140	0.00091	0.00100
oh	0.19082	0.00077	0.00286	0.00273	0.00286	0.00117	0.00089	0.00110	0.00046	0.00012	0.00036	0.00019	0.00062	0.00040	0.00015	0.00022	0.00004
ch2–trip	0.88953	0.05021	0.41814	0.41809	0.41807	0.14599	0.14599	0.14610	0.03140	0.03142	0.03158	0.01311	0.01307	0.01295	0.01885	0.01882	0.01863
nh	0.14952	0.00304	0.02496	0.02500	0.02508	0.00885	0.00879	0.00885	0.00207	0.00197	0.00201	0.00092	0.00108	0.00103	0.00091	0.00103	0.00099
		MAX	0.79286	0.79310	0.79316	0.27634	0.27679	0.27718	0.05886	0.05940	0.05992	0.02563	0.02497	0.02459	0.03650	0.03593	0.03534
		MAD	0.19875	0.19881	0.19877	0.06915	0.06933	0.06938	0.01458	0.01481	0.01490	0.00627	0.00599	0.00592	0.00938	0.00910	0.00899
		RMS	0.32391	0.32398	0.32397	0.11288	0.11304	0.11319	0.02403	0.02423	0.02444	0.01037	0.01012	0.00997	0.01495	0.01472	0.01448
		SD	0.26961	0.26964	0.26967	0.09405	0.09411	0.09427	0.02013	0.02021	0.02042	0.00871	0.00860	0.00846	0.01226	0.01220	0.01196

Table S6. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. Reference values are computed as the mean of SDTQ(P)/eN{D,T}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	SDTQ/DZ – SDT(Q)/TZ	SDTQ(P)/DZ – SDTQ/TZ
bh3	0.51676	0.51637
ch2–sing	0.09981	0.09980
h2o	0.03212	0.03101
hf	0.01794	0.01725
ch	0.02537	0.02554
ch3	0.30362	0.30331
nh2	0.01125	0.01076
oh	0.00156	0.00197
ch2–trip	0.27210	0.27208
nh	0.01615	0.01629
MAX	0.51676	0.51637
MAD	0.12967	0.12944
RMS	0.21109	0.21093
SD	0.17559	0.17555

Table S7. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SDTQP/eN{D,T}Z (N = 1 – 3) values. The range of SDTQP/eN{D,T}Z (N = 1 – 3) values (RANGE, RMS = 0.0486 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SDTQ(P)/DZ	SDTQP/DZ	SDTQ(P)/TZ	SDTQP/TZ	SDTQ(P)/e1{D,T}Z	SDTQP/e1{D,T}Z	SDTQ(P)/e2{D,T}Z	SDTQP/e2{D,T}Z	SDTQ(P)/e3{D,T}Z	SDTQP/e3{D,T}Z
bh3	1.26812	0.09529	0.79342	0.79336	0.27744	0.27723	0.06019	0.05991	0.02432	0.02453	0.03508	0.03538
ch2-sing	0.49932	0.01842	0.15297	0.15282	0.05353	0.05305	0.01166	0.01104	0.00318	0.00366	0.00670	0.00738
h2o	0.46202	0.00583	0.04819	0.04821	0.01665	0.01661	0.00338	0.00331	0.00073	0.00078	0.00245	0.00253
hf	0.22761	0.00325	0.02686	0.02686	0.00927	0.00927	0.00186	0.00186	0.00047	0.00047	0.00139	0.00139
		MAX	0.79342	0.79336	0.27744	0.27723	0.06019	0.05991	0.02432	0.02453	0.03508	0.03538
		MAD	0.25536	0.25531	0.08922	0.08904	0.01927	0.01903	0.00718	0.00736	0.01140	0.01167
		RMS	0.40496	0.40491	0.14160	0.14145	0.03071	0.03052	0.01227	0.01241	0.01791	0.01813
		SD	0.36292	0.36290	0.12696	0.12691	0.02762	0.02755	0.01150	0.01154	0.01595	0.01602

Table S8. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. Reference values are computed as the mean of SDTQP/eN{D,T}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	$\frac{\text{SDTQP/DZ}}{\text{SDTQP/TZ}}$
bh3	0.51592
ch2-sing	0.09929
h2o	0.03155
hf	0.01759
MAX	0.51592
MAD	0.16609
RMS	0.26331
SD	0.23593

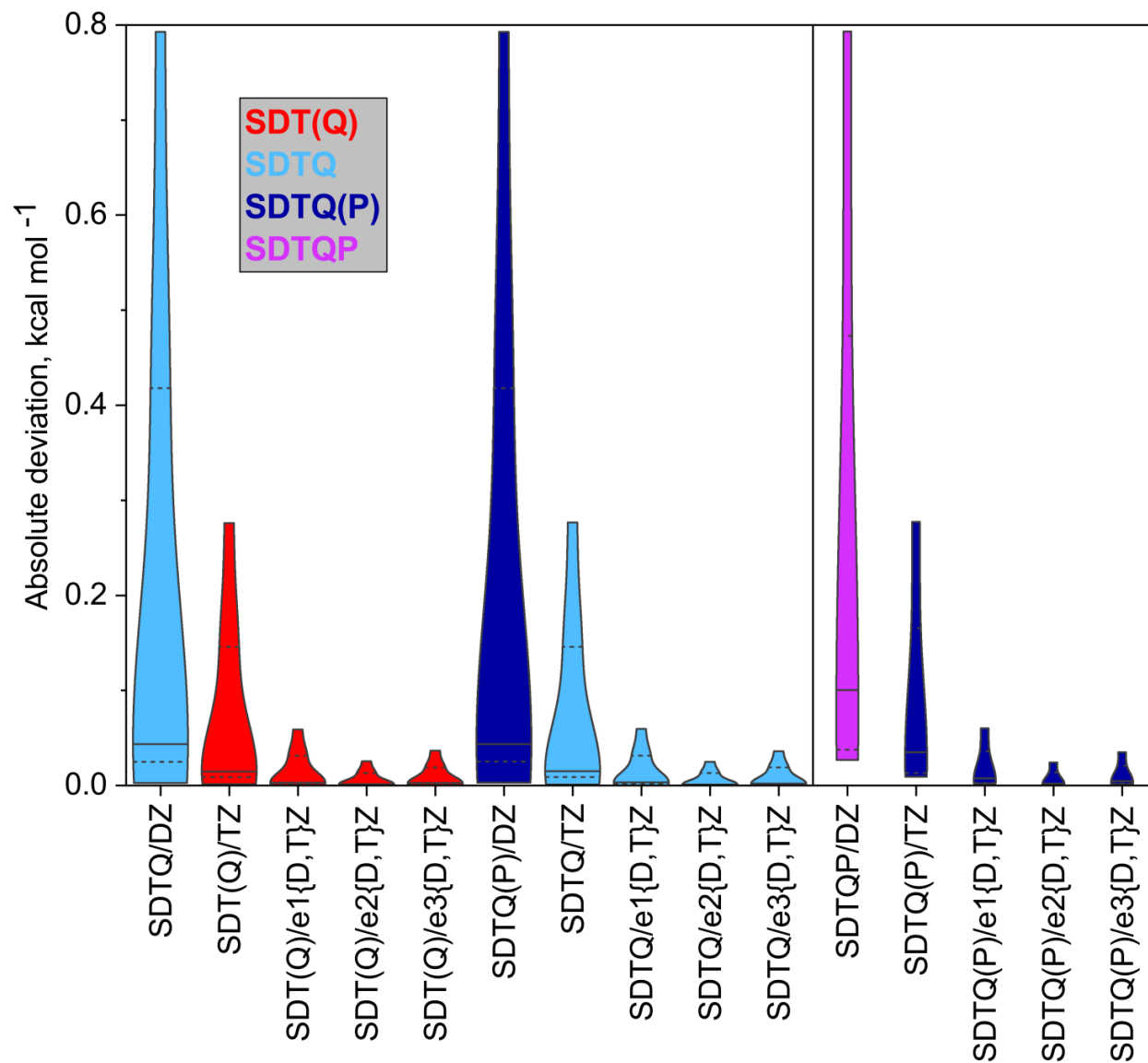


Figure S7. Violin plots of the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SDTQ(P) (left panel) or SDTQP (right panel) $eN\{D,T\}Z$ ($N = 1 - 3$) values. The median (solid), 25th, and 75th percentiles (dash) are shown. The highest point of a plot represents the maximum deviation.

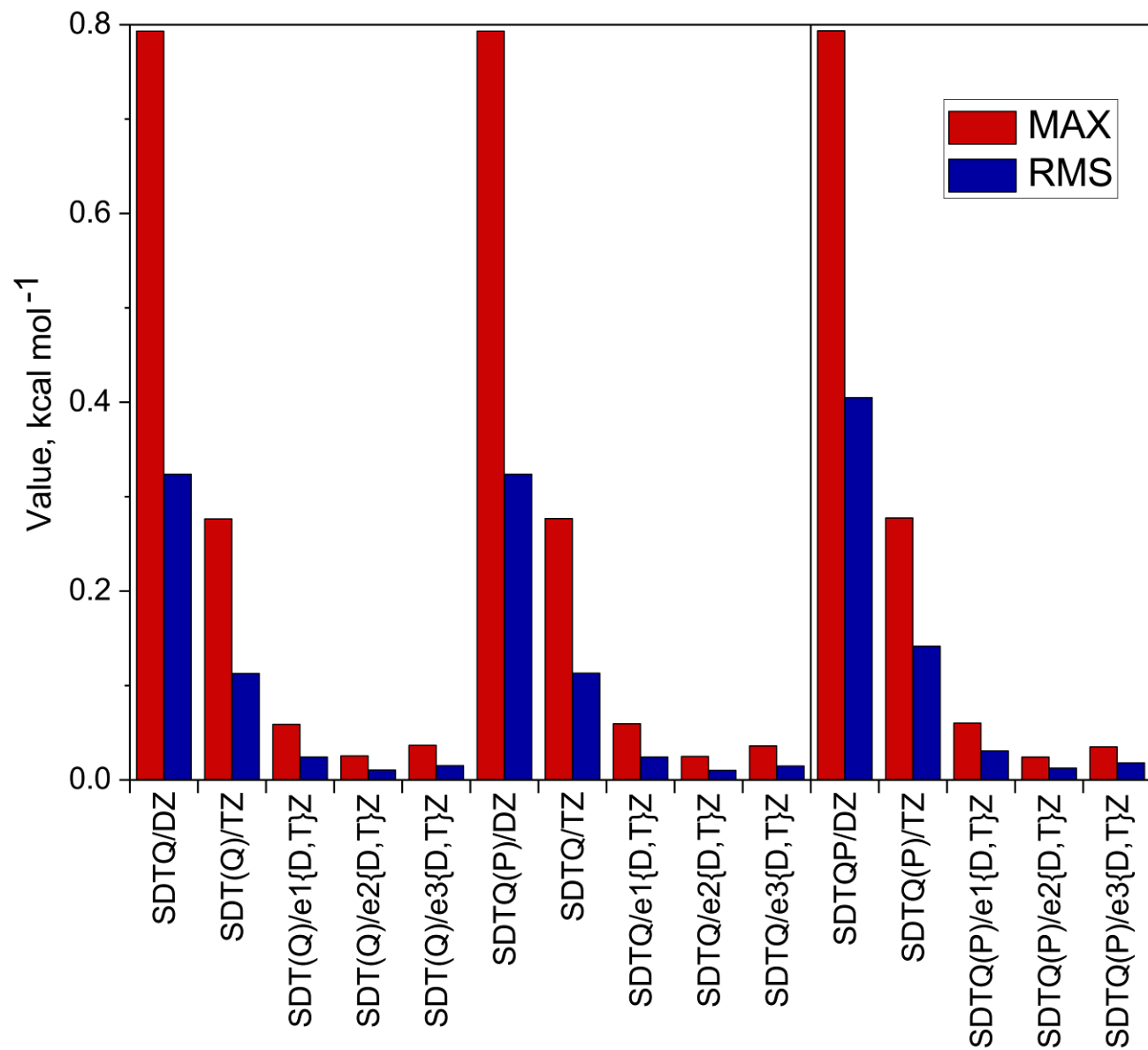


Figure S8. Maximum (MAX) and root mean square (RMS) values for the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SDTQ(P) (left panel) or SDTQP (right panel) eN{D,T}Z (N = 1 – 3) values.

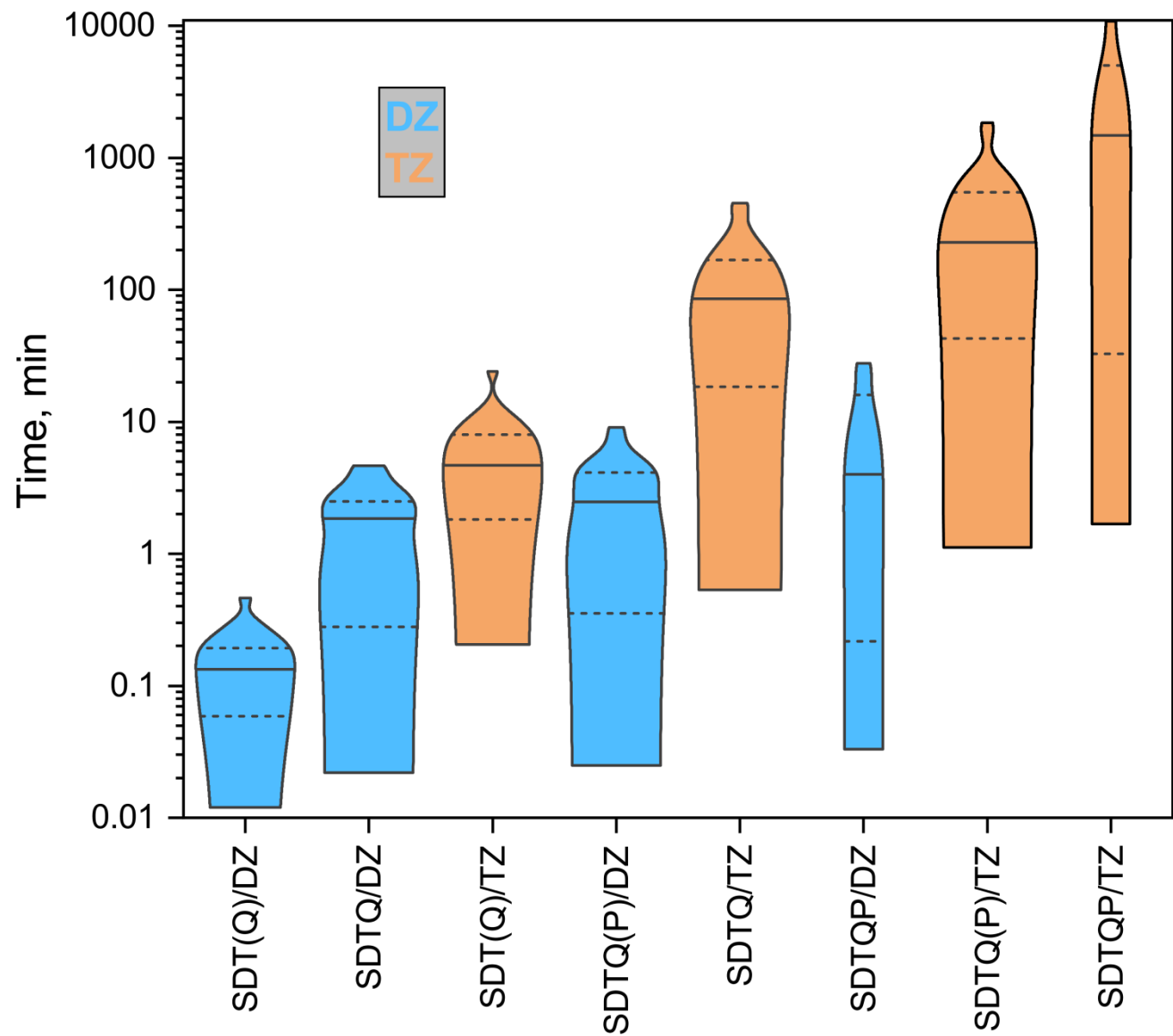


Figure S9. Computational times for different levels of theory. The times for the FC and CV calculations were combined and used for the visualization. The median (solid), 25th, and 75th percentiles (dash) are shown.

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Table S9. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SDT(Q)/eN{aT,aQ}Z (N = 1 – 3) values. The range of SDT(Q)/eN{aT,aQ}Z (N = 1 – 3) values (RANGE, RMS = 0.0048 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SD(T)/aDZ	SDT/aDZ	SDT(Q)/aDZ	SD(T)/aTZ	SDT/aTZ	SDT(Q)/aTZ	SD(T)/aQZ	SDT/aQZ	SDT(Q)/aQZ	SD(T)/e1{aD,aT}Z	SDT/e1{aD,aT}Z	SD(T)/e1{aT,aQ}Z	SDT/e1{aT,aQ}Z	SDT(Q)/e1{aT,aQ}Z	SD(T)/e2{aD,aT}Z	SDT/e2{aD,aT}Z	SDT(Q)/e2{aD,aT}Z	SD(T)/e2{aT,aQ}Z	SDT/e2{aT,aQ}Z	SDT(Q)/e2{aT,aQ}Z	SD(T)/e3{aD,aT}Z	SDT/e3{aD,aT}Z	SDT(Q)/e3{aD,aT}Z	SD(T)/e3{aT,aQ}Z	SDT/e3{aT,aQ}Z	SDT(Q)/e3{aT,aQ}Z	
alh	-0.0789	0.0033	0.0855	0.0996	0.0934	0.0094	0.0380	0.0252	0.0043	0.0253	0.0110	0.0227	0.0120	0.0035	0.0143	0.0161	0.0006	0.0337	0.0021	0.0134	0.0140	0.0166	0.0013	0.0367	0.0006	0.0161	0.0168	0.0138	0.0020
bh	0.2304	0.0029	0.0865	0.0814	0.0831	0.0391	0.0258	0.0281	0.0248	0.0101	0.0124	0.0191	0.0024	0.0049	0.0143	0.0013	0.0010	0.0122	0.0051	0.0026	0.0146	0.0014	0.0009	0.0104	0.0079	0.0052	0.0117	0.0042	0.0019
ch2-sing	0.5016	0.0043	0.1085	0.0958	0.0953	0.0748	0.0420	0.0417	0.0559	0.0191	0.0185	0.0606	0.0194	0.0191	0.0421	0.0024	0.0016	0.0558	0.0130	0.0127	0.0425	0.0018	0.0011	0.0544	0.0095	0.0092	0.0387	0.0018	0.0027
h2o	0.4897	0.0037	0.0629	0.0654	0.0604	0.0444	0.0417	0.0358	0.0272	0.0222	0.0158	0.0367	0.0318	0.0254	0.0146	0.0079	0.0013	0.0340	0.0287	0.0223	0.0149	0.0077	0.0011	0.0332	0.0274	0.0208	0.0114	0.0043	0.0024
hcl	0.2460	0.0080	0.0090	0.0185	0.0148	0.0686	0.0612	0.0661	0.0288	0.0236	0.0290	0.1012	0.0947	0.1001	0.0002	0.0038	0.0019	0.1124	0.1061	0.1115	0.0005	0.0026	0.0031	0.1155	0.1094	0.1151	0.0076	0.0107	0.0050
hf	0.2353	0.0015	0.0278	0.0302	0.0267	0.0163	0.0196	0.0140	0.0095	0.0123	0.0062	0.0114	0.0151	0.0086	0.0046	0.0070	0.0005	0.0097	0.0135	0.0070	0.0047	0.0069	0.0005	0.0093	0.0132	0.0063	0.0033	0.0056	0.0010
ch	0.1958	0.0011	0.0090	0.0056	0.0057	0.0225	0.0108	0.0111	0.0179	0.0048	0.0049	0.0282	0.0130	0.0134	0.0146	0.0004	0.0005	0.0301	0.0143	0.0147	0.0147	0.0001	0.0002	0.0307	0.0139	0.0144	0.0137	0.0008	0.0007
hs	0.2219	0.0065	0.0034	0.0089	0.0095	0.0527	0.0542	0.0535	0.0209	0.0242	0.0235	0.0763	0.0808	0.0801	0.0024	0.0023	0.0015	0.0844	0.0895	0.0887	0.0018	0.0033	0.0025	0.0867	0.0925	0.0917	0.0082	0.0032	0.0040
nh2	0.4369	0.0032	0.0192	0.0192	0.0168	0.0426	0.0333	0.0315	0.0273	0.0159	0.0140	0.0524	0.0393	0.0377	0.0162	0.0032	0.0012	0.0558	0.0420	0.0404	0.0165	0.0029	0.0009	0.0567	0.0419	0.0404	0.0134	0.0001	0.0021
oh	0.2078	0.0012	0.0010	0.0002	0.0022	0.0163	0.0155	0.0121	0.0109	0.0091	0.0053	0.0236	0.0219	0.0181	0.0069	0.0044	0.0004	0.0262	0.0242	0.0204	0.0070	0.0043	0.0004	0.0268	0.0247	0.0207	0.0059	0.0032	0.0008
sih	0.0511	0.0040	0.0031	0.0062	0.0010	0.0181	0.0410	0.0317	0.0003	0.0242	0.0139	0.0244	0.0556	0.0447	0.0126	0.0120	0.0009	0.0266	0.0593	0.0484	0.0123	0.0126	0.0016	0.0272	0.0620	0.0504	0.0159	0.0089	0.0024
ch2-trip	0.8526	0.0106	0.3198	0.3201	0.3226	0.0940	0.0920	0.0956	0.0409	0.0382	0.0421	0.0011	0.0041	0.0001	0.0022	0.0011	0.0030	0.0339	0.0370	0.0328	0.0032	0.0003	0.0038	0.0428	0.0462	0.0418	0.0076	0.0110	0.0068
nh	0.1699	0.0008	0.0300	0.0298	0.0308	0.0130	0.0085	0.0076	0.0098	0.0044	0.0034	0.0310	0.0247	0.0238	0.0075	0.0014	0.0003	0.0372	0.0305	0.0297	0.0075	0.0013	0.0002	0.0390	0.0317	0.0309	0.0069	0.0007	0.0005
		MAX	0.3198	0.3201	0.3226	0.0940	0.0920	0.0956	0.0559	0.0382	0.0421	0.1012	0.0947	0.1001	0.0421	0.0161	0.0030	0.1124	0.1061	0.1115	0.0425	0.0166	0.0038	0.1155	0.1094	0.1151	0.0387	0.0138	0.0068
		MAD	0.0589	0.0601	0.0586	0.0394	0.0372	0.0349	0.0214	0.0180	0.0154	0.0376	0.0319	0.0292	0.0117	0.0049	0.0011	0.0425	0.0358	0.0342	0.0119	0.0047	0.0013	0.0438	0.0370	0.0356	0.0124	0.0053	0.0025
		RMS	0.1019	0.1020	0.1018	0.0471	0.0433	0.0424	0.0260	0.0202	0.0187	0.0462	0.0422	0.0412	0.0156	0.0067	0.0013	0.0507	0.0471	0.0462	0.0157	0.0067	0.0017	0.0522	0.0489	0.0480	0.0150	0.0068	0.0030
		SD	0.0866	0.0857	0.0866	0.0269	0.0230	0.0250	0.0154	0.0097	0.0110	0.0280	0.0288	0.0302	0.0107	0.0047	0.0008	0.0288	0.0319	0.0324	0.0108	0.0050	0.0011	0.0296	0.0334	0.0336	0.0089	0.0045	0.0018

Table S10. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. Reference values are computed as the mean of SDT(Q)/eN{aT,aQ}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	$\frac{\text{SDT/aDZ}}{\text{SD(T)/aTZ}}$	$\frac{\text{SDT(Q)/aDZ}}{\text{SD(T)/aTZ}}$	$\frac{\text{SDT/aTZ}}{\text{SD(T)/aQZ}}$	$\frac{\text{SDT(Q)/aTZ}}{\text{SD(T)/aQZ}}$	$\frac{\text{SDT/e1\{aD,aT\}Z}}{\text{SD(T)/e1\{aT,aQ\}Z}}$	$\frac{\text{SDT(Q)/e1\{aD,aT\}Z}}{\text{SD(T)/e1\{aT,aQ\}Z}}$	$\frac{\text{SDT/e2\{aD,aT\}Z}}{\text{SD(T)/e2\{aT,aQ\}Z}}$	$\frac{\text{SDT(Q)/e2\{aD,aT\}Z}}{\text{SD(T)/e2\{aT,aQ\}Z}}$	$\frac{\text{SDT/e3\{aD,aT\}Z}}{\text{SD(T)/e3\{aT,aQ\}Z}}$	$\frac{\text{SDT(Q)/e3\{aD,aT\}Z}}{\text{SD(T)/e3\{aT,aQ\}Z}}$
alh	0.0902	0.0555	0.0337	-0.0001	-0.0022	-0.0126	-0.0119	-0.0032	-0.0161	0.0023
bh	0.0423	0.0573	0.0010	0.0180	-0.0119	0.0036	-0.0094	0.0012	-0.0038	0.0010
ch2–sing	0.0210	0.0532	-0.0139	0.0225	-0.0228	0.0167	-0.0295	0.0108	-0.0292	0.0074
h2o	0.0210	0.0187	0.0145	0.0136	0.0172	0.0175	0.0138	0.0146	0.0160	0.0165
hcl	-0.0501	-0.0463	0.0324	0.0425	0.0945	0.0963	0.1056	0.1089	0.1018	0.1043
hf	0.0140	0.0071	0.0101	0.0017	0.0105	0.0016	0.0088	0.0000	0.0098	0.0006
ch	-0.0169	-0.0051	-0.0071	0.0063	-0.0016	0.0130	-0.0004	0.0146	0.0002	0.0136
hs	-0.0438	-0.0448	0.0334	0.0293	0.0784	0.0778	0.0877	0.0854	0.0842	0.0885
nh2	-0.0234	-0.0165	0.0060	0.0156	0.0231	0.0345	0.0255	0.0375	0.0285	0.0404
oh	-0.0161	-0.0132	0.0046	0.0030	0.0150	0.0137	0.0173	0.0162	0.0188	0.0175
sih	-0.0119	-0.0400	0.0406	0.0075	0.0430	0.0327	0.0470	0.0358	0.0461	0.0414
ch2–trip	0.2262	0.2307	0.0510	0.0575	0.0019	-0.0010	0.0339	0.0326	0.0387	0.0309
nh	0.0168	0.0223	-0.0013	0.0032	0.0172	0.0224	0.0230	0.0284	0.0248	0.0302
MAX	0.2262	0.2307	0.0360	0.0575	0.0526	0.0840	0.0636	0.0949	0.0707	0.1013
MAD	0.0207	0.0214	0.0158	0.0170	0.0202	0.0243	0.0239	0.0295	0.0246	0.0304
RMS	0.0549	0.0585	0.0173	0.0221	0.0266	0.0345	0.0314	0.0395	0.0339	0.0413
SD	0.0588	0.0636	0.0076	0.0153	0.0181	0.0255	0.0211	0.0274	0.0245	0.0291

Table S11. Computational times for coupled-cluster calculations with augmented basis sets, in min. System name (System), anZ basis set cardinal number (Cardinal), and times for the computations using optimized CCSD(T) program “ccsd” or string-based CC program “mrcc” are provided.

System	Cardinal	Optimized CCSD(T)	Automated string-based CCSD(T)	Automated string-based CCSDT	Automated string-based CCSDT(Q)
Al	2	0.014	0.033	0.311	0.453
alh	2	0.007	0.115	1.177	1.586
B	2	0.007	0.014	0.031	0.04
bh	2	0.003	0.049	0.132	0.167
C	2	0.007	0.013	0.034	0.043
ch	2	0.017	0.064	0.266	0.33
ch2-sing	2	0.007	0.13	0.592	0.795
ch2-trip	2	0.036	0.147	0.605	0.846
Cl	2	0.017	0.04	0.628	0.894
F	2	0.007	0.016	0.088	0.118
h2o	2	0.007	0.133	0.853	1.206
hcl	2	0.009	0.119	1.953	2.671
hf	2	0.005	0.057	0.366	0.479
hs	2	0.035	0.159	2.834	3.627
N	2	0.006	0.012	0.037	0.048
nh	2	0.017	0.07	0.326	0.408
nh2	2	0.041	0.177	1.059	1.416
O	2	0.007	0.02	0.08	0.117
oh	2	0.017	0.078	0.464	0.584
P	2	0.013	0.033	0.359	0.521
S	2	0.015	0.047	0.66	1.033
Si	2	0.014	0.039	0.431	0.709
sih	2	0.036	0.158	2.112	2.704
Al	3	0.241	0.48	4.223	14.415
alh	3	0.072	2.205	16.476	41.813
B	3	0.1	0.202	0.403	0.717
bh	3	0.03	1.145	2.511	4.211
C	3	0.093	0.188	0.477	0.821
ch	3	0.446	1.587	4.821	8.063
ch2-sing	3	0.092	3.313	10.604	23.886
ch2-trip	3	1.141	3.897	12.139	28.503

System	Cardinal	Optimized CCSD(T)	Automated string-based CCSD(T)	Automated string-based CCSDT	Automated string-based CCSDT(Q)
Cl	3	0.233	0.618	9.778	29.695
F	3	0.101	0.217	1.157	2.484
h2o	3	0.094	3.104	15.048	38.587
hcl	3	0.096	2.15	31.985	85.444
hf	3	0.038	1.155	5.863	12.336
hs	3	0.796	3.029	47.243	104.614
N	3	0.092	0.176	0.487	0.937
nh	3	0.449	1.549	5.591	9.955
nh2	3	1.265	4.107	19.056	43.018
O	3	0.1	0.269	1.076	2.692
oh	3	0.436	1.637	7.911	14.32
P	3	0.21	0.443	4.525	11.408
S	3	0.245	0.639	8.315	25.226
Si	3	0.229	0.577	5.369	17.375
sih	3	0.858	2.943	33.702	73.271
Al	4	2.659	4.482	33.04	199.558
alh	4	0.638	23.346	199.723	934.996
B	4	1.243	2.028	3.664	8.546
bh	4	0.304	13.612	26.089	70.991
C	4	1.237	2.165	4.576	13.034
ch	4	5.815	20.224	61.084	222.772
ch2-sing	4	0.951	41.825	131.488	587.681
ch2-trip	4	15.838	56.195	171.765	750.704
Cl	4	2.516	5.179	70.873	415.569
F	4	1.204	2.152	8.902	32.449
h2o	4	0.93	38.338	195.065	1017.751
hcl	4	0.706	22.366	387.072	1981.593
hf	4	0.363	12.525	62.579	253.012
hs	4	9.689	35.22	701.283	3192.258
N	4	1.118	1.88	4.266	11.983
nh	4	5.804	17.586	61.339	189.065
nh2	4	17.476	65.175	320.395	1736.788
O	4	1.316	2.478	8.222	36.497

System	Cardinal	Optimized CCSD(T)	Automated string-based CCSD(T)	Automated string-based CCSDT	Automated string-based CCSDT(Q)
oh	4	5.803	20.598	105.367	451.34
P	4	2.385	4.112	34.818	162.057
S	4	2.763	5.083	63.269	342.929
Si	4	2.45	4.696	39.187	233.158
sih	4	10.388	36.112	494.864	2236.11

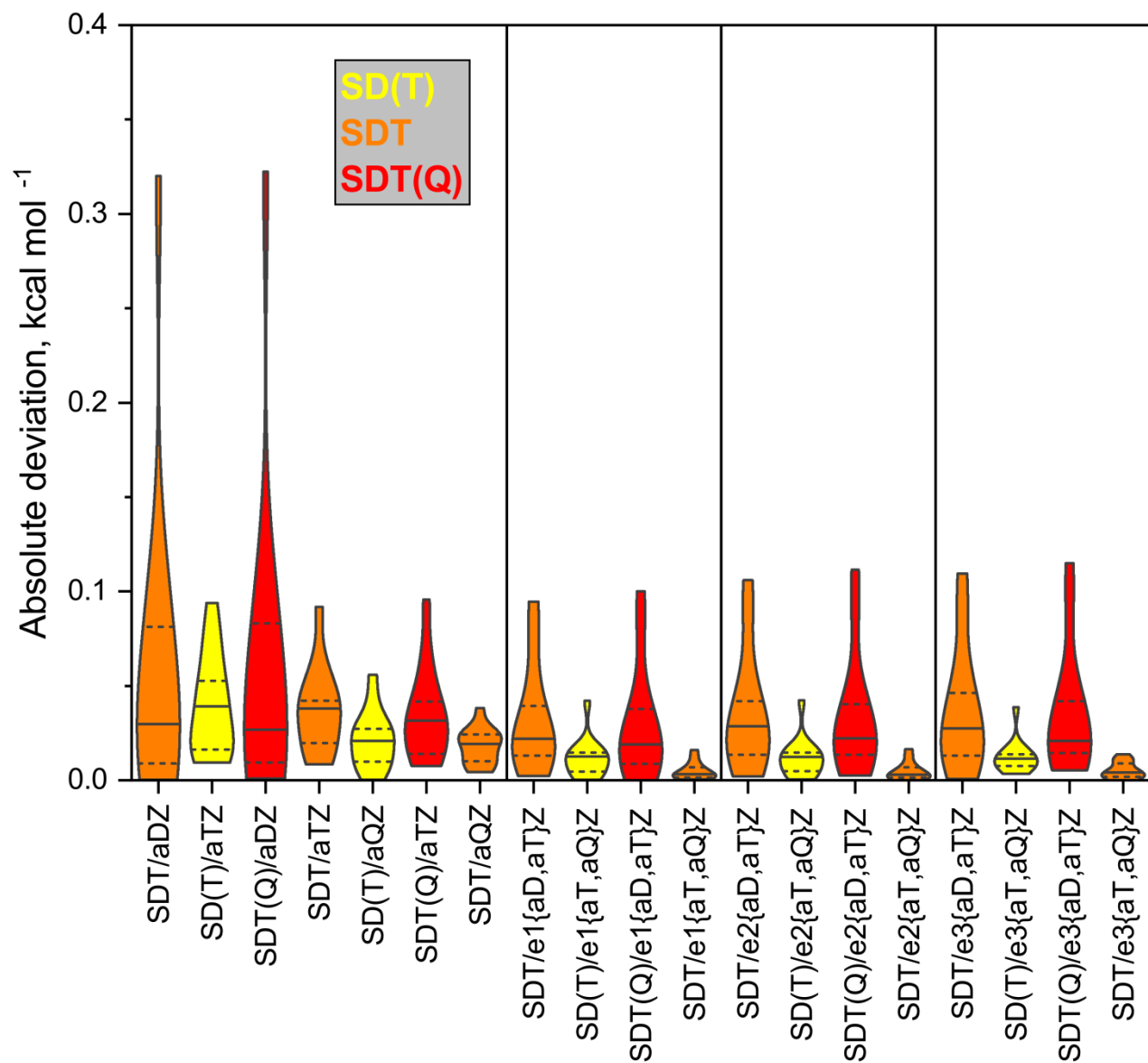


Figure S10. Violin plots of the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SDT(Q)/eN{aT,aQ}Z (N = 1 – 3) values. The median (solid), 25th, and 75th percentiles (dash) are shown. The highest point of a plot represents the maximum deviation.

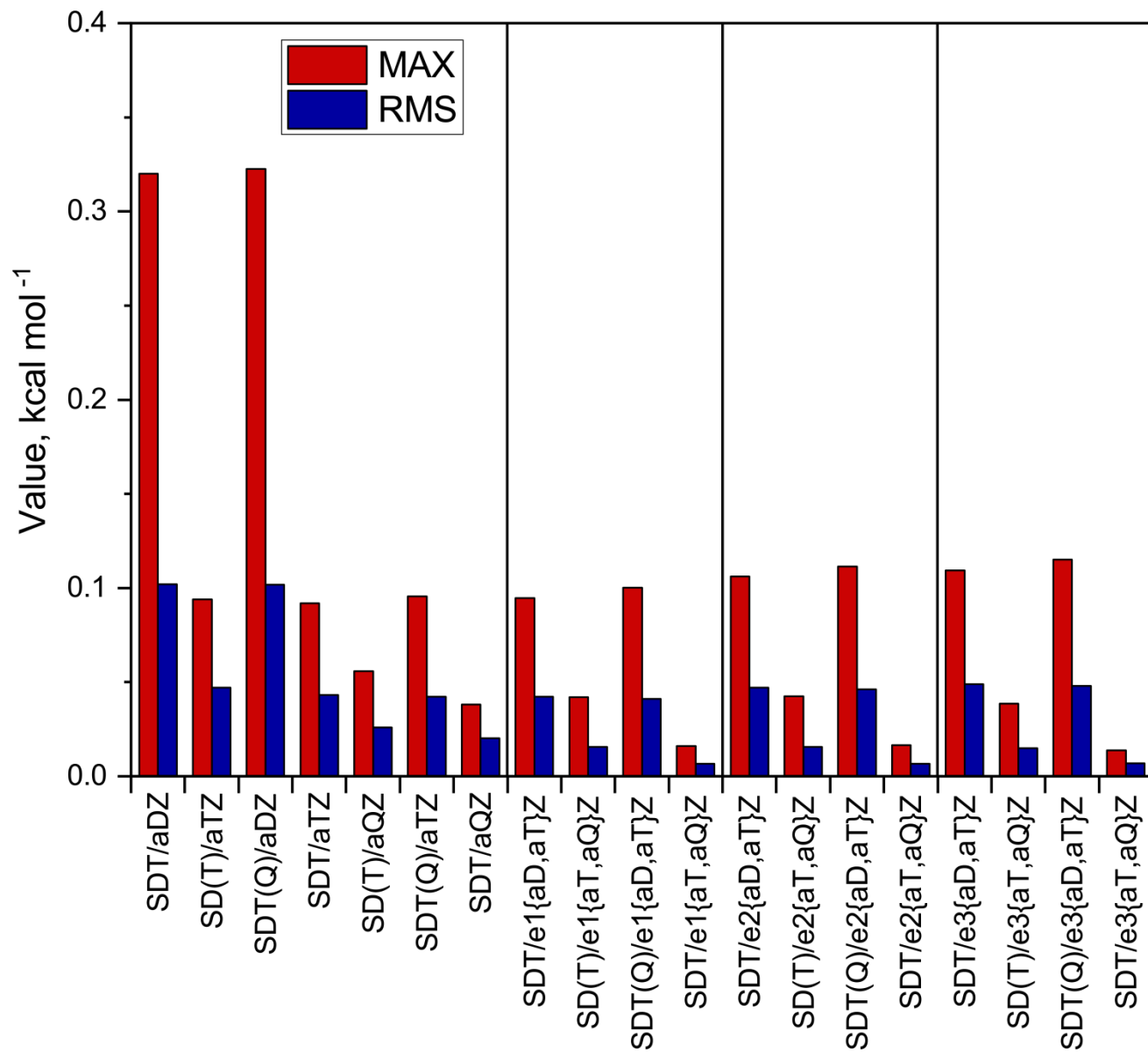


Figure S11. Maximum (MAX) and root mean square (RMS) values for the absolute deviations obtained at a given level of theory. Reference values are computed as the mean of SDT(Q)/eN{aT,aQ}Z (N = 1 – 3) values.

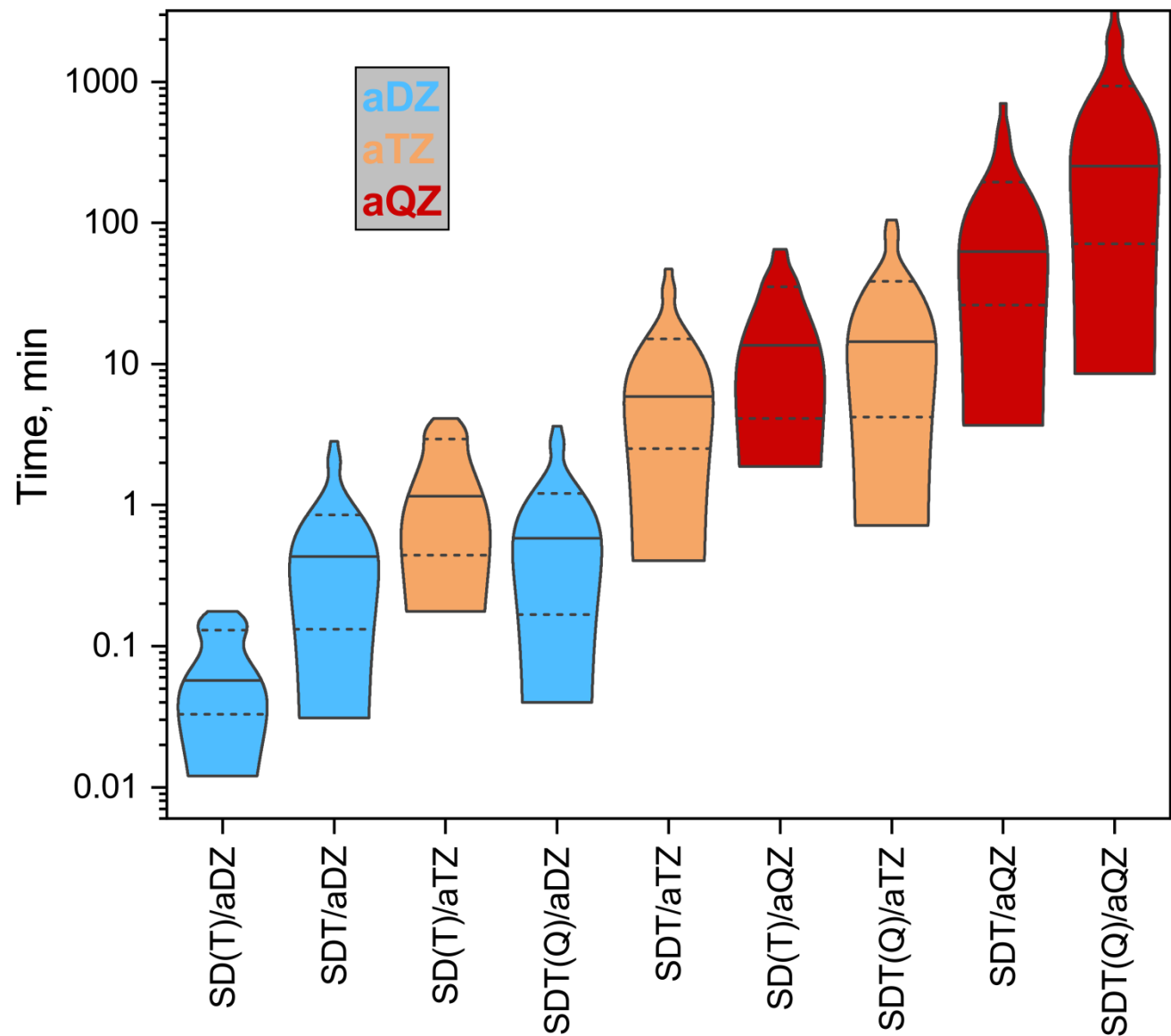


Figure S12. Computational times for different levels of theory. The times for the FC and CV calculations were combined and used for the visualization. The data for the SD(T) method were obtained using the string-based CC program “mrcc” for systems for which SDT(Q) computations were performed. The median (solid), 25th, and 75th percentiles (dash) are shown.

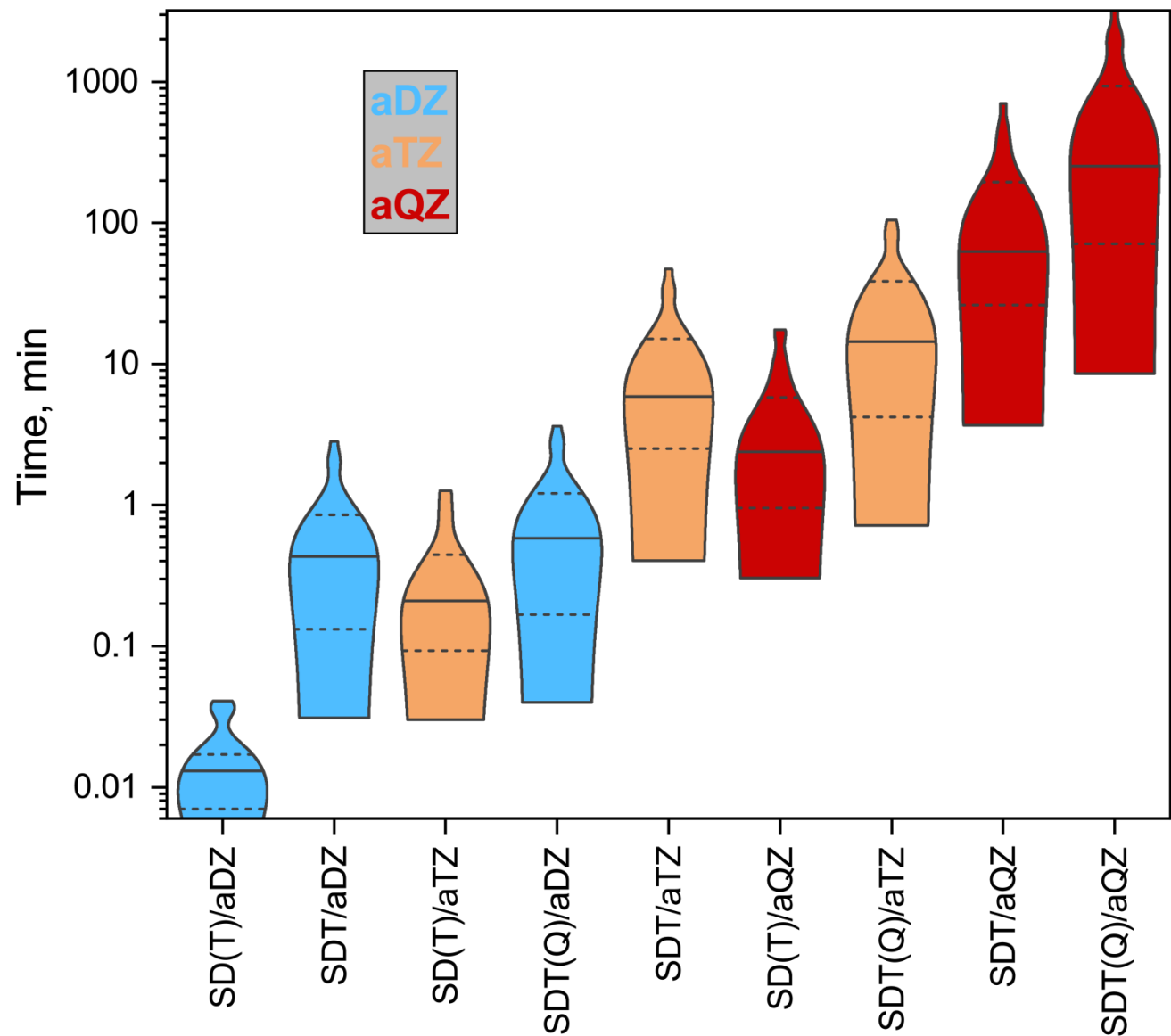


Figure S13. Computational times for different levels of theory. The times for the FC and CV calculations were combined and used for the visualization. The data for the SD(T) method were obtained using the optimized CCSD(T) program “ccsd” for systems for which SDT(Q) computations were performed. The median (solid), 25th, and 75th percentiles (dash) are shown.

Batch #6

Table S12. Absolute deviations of core-valence corrections to the atomization energy from reference values in kcal mol⁻¹. Reference values (REFERENCE) are computed as the mean of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values. The geometries were optimized using SD(T)/nZ method with the basis set and frozen core approximation type corresponding to the given energy evaluation (FC-SD(T) for the FC component of core-valence correction and CV-SD(T) for the CV one). The range of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values (RANGE, RMS = 0.0106 kcal mol⁻¹) and the absolute deviations for a given coupled-cluster method and basis set (including extrapolated results) are shown. Color encoding shows the highest (red) and the lowest (green) values. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	REFERENCE	RANGE	SD(T)/DZ	SDT/DZ	SDT(Q)/DZ	SD(T)/TZ	SDT/TZ	SDT(Q)/TZ	SD(T)/QZ	SDT/QZ	SDT(Q)/QZ	SD(T)/e1{D,T}Z	SDT/e1{D,T}Z	SDT(Q)/e1{D,T}Z	SD(T)/e1{T,Q}Z	SDT/e1{T,Q}Z	SDT(Q)/e1{T,Q}Z	SD(T)/e2{D,T}Z	SDT/e2{D,T}Z	SDT(Q)/e2{D,T}Z	SD(T)/e2{T,Q}Z	SDT/e2{T,Q}Z	SDT(Q)/e2{T,Q}Z	SD(T)/e3{D,T}Z	SDT/e3{D,T}Z	SDT(Q)/e3{D,T}Z	SD(T)/e3{T,Q}Z	SDT/e3{T,Q}Z	SDT(Q)/e3{T,Q}Z
alh	-0.0701	0.0047	0.1856	0.1725	0.1771	0.0620	0.0348	0.0469	0.0355	0.0062	0.0206	0.0102	0.0230	0.0077	0.0166	0.0143	0.0017	0.0096	0.0439	0.0286	0.0170	0.0144	0.0014	0.0122	0.0480	0.0313	0.0118	0.0195	0.0030
bf	0.8503	0.0186	0.4681	0.4609	0.4559	0.2123	0.1963	0.1889	0.1057	0.0866	0.0795	0.1097	0.0899	0.0816	0.0338	0.0125	0.0056	0.0766	0.0561	0.0478	0.0354	0.0135	0.0065	0.0723	0.0508	0.0420	0.0166	0.0052	0.0121
bh	0.2343	0.0039	0.1489	0.1444	0.1457	0.0499	0.0371	0.0393	0.0290	0.0147	0.0170	0.0090	0.0072	0.0047	0.0144	0.0011	0.0013	0.0057	0.0225	0.0200	0.0147	0.0011	0.0013	0.0076	0.0254	0.0227	0.0108	0.0050	0.0026
bh3	1.1811	0.0214	0.7185	0.7174	0.7222	0.1862	0.1837	0.1905	0.0808	0.0769	0.0843	0.0380	0.0410	0.0335	0.0032	0.0018	0.0061	0.1250	0.1281	0.1205	0.0051	0.0002	0.0076	0.1363	0.1396	0.1317	0.0166	0.0218	0.0138
ch2-sing	0.5126	0.0067	0.2021	0.1891	0.1884	0.1029	0.0690	0.0688	0.0680	0.0301	0.0297	0.0621	0.0195	0.0195	0.0437	0.0030	0.0023	0.0476	0.0034	0.0034	0.0443	0.0026	0.0020	0.0458	0.0007	0.0006	0.0378	0.0037	0.0044
co	1.2042	0.0202	0.5853	0.5819	0.5687	0.2615	0.2336	0.2212	0.1364	0.1032	0.0913	0.1352	0.0970	0.0849	0.0550	0.0179	0.0064	0.0996	0.0594	0.0474	0.0569	0.0185	0.0069	0.0949	0.0521	0.0402	0.0362	0.0019	0.0133
f2	0.0493	0.0050	0.0410	0.0497	0.0584	0.0242	0.0122	0.0152	0.0349	0.0071	0.0097	0.0548	0.0068	0.0061	0.0478	0.0018	0.0005	0.0709	0.0207	0.0200	0.0474	0.0001	0.0022	0.0730	0.0198	0.0202	0.0519	0.0049	0.0027
h2o	0.4953	0.0052	0.0973	0.0978	0.0945	0.0623	0.0566	0.0525	0.0335	0.0269	0.0220	0.0486	0.0404	0.0358	0.0143	0.0070	0.0015	0.0446	0.0360	0.0314	0.0147	0.0072	0.0018	0.0441	0.0348	0.0301	0.0098	0.0023	0.0033
h2s	0.4458	0.0052	0.1828	0.1952	0.1940	0.0275	0.0293	0.0281	0.0110	0.0162	0.0142	0.1143	0.1220	0.1198	0.0042	0.0034	0.0009	0.1456	0.1544	0.1522	0.0037	0.0046	0.0022	0.1497	0.1600	0.1573	0.0086	0.0004	0.0031
hcl	0.2615	0.0019	0.0820	0.0923	0.0896	0.0102	0.0034	0.0076	0.0047	0.0003	0.0045	0.0483	0.0430	0.0478	0.0011	0.0049	0.0003	0.0623	0.0572	0.0621	0.0010	0.0043	0.0008	0.0641	0.0594	0.0646	0.0030	0.0064	0.0011
hf	0.2375	0.0020	0.0393	0.0402	0.0378	0.0223	0.0233	0.0188	0.0115	0.0130	0.0076	0.0157	0.0166	0.0113	0.0045	0.0065	0.0004	0.0137	0.0147	0.0093	0.0047	0.0068	0.0008	0.0135	0.0144	0.0087	0.0030	0.0051	0.0012
n2	1.1430	0.0146	0.5022	0.4963	0.4836	0.2373	0.1886	0.1858	0.1316	0.0739	0.0731	0.1392	0.0724	0.0737	0.0687	0.0044	0.0052	0.1186	0.0486	0.0499	0.0700	0.0037	0.0042	0.1160	0.0413	0.0444	0.0553	0.0106	0.0094
nh3	0.8139	0.0099	0.2112	0.2098	0.2072	0.1146	0.0994	0.0988	0.0616	0.0434	0.0426	0.0750	0.0540	0.0542	0.0245	0.0041	0.0032	0.0610	0.0389	0.0391	0.0254	0.0043	0.0034	0.0591	0.0356	0.0362	0.0154	0.0055	0.0065
cf	0.4542	0.0045	0.1243	0.1225	0.1151	0.0780	0.0662	0.0551	0.0474	0.0336	0.0220	0.0616	0.0456	0.0329	0.0289	0.0135	0.0015	0.0592	0.0424	0.0298	0.0293	0.0134	0.0015	0.0589	0.0410	0.0277	0.0248	0.0091	0.0030
ch	0.2014	0.0024	0.0630	0.0597	0.0598	0.0363	0.0247	0.0253	0.0233	0.0104	0.0108	0.0255	0.0106	0.0113	0.0146	0.0006	0.0008	0.0221	0.0065	0.0073	0.0148	0.0004	0.0007	0.0216	0.0052	0.0060	0.0125	0.0018	0.0016
ch3	1.1457	0.0160	0.4735	0.4724	0.4736	0.1511	0.1445	0.1483	0.0687	0.0604	0.0648	0.0157	0.0067	0.0116	0.0094	0.0001	0.0047	0.0364	0.0459	0.0409	0.0109	0.0010	0.0057	0.0432	0.0533	0.0479	0.0054	0.0152	0.0104
cn	1.4262	0.0237	0.7158	0.6987	0.6748	0.3118	0.2543	0.2354	0.1838	0.1197	0.1017	0.1474	0.0729	0.0561	0.0938	0.0249	0.0076	0.0913	0.0137	0.0032	0.0960	0.0255	0.0081	0.0839	0.0020	0.0140	0.0717	0.0015	0.0156
hs	0.2239	0.0031	0.0743	0.0814	0.0821	0.0190	0.0207	0.0194	0.0078	0.0108	0.0094	0.0573	0.0626	0.0611	0.0020	0.0020	0.0006	0.0708	0.0768	0.0752	0.0018	0.0026	0.0012	0.0725	0.0795	0.0778	0.0048	0.0005	0.0019

System	REFERENCE	RANGE	SD(T)/DZ	SDT/DZ	SDT(Q)/DZ	SD(T)/TZ	SDT/TZ	SDT(Q)/TZ	SD(T)/QZ	SDT/QZ	SDT(Q)/QZ	SD(T)/e1{D,T}Z	SDT/e1{D,T}Z	SDT(Q)/e1{D,T}Z	SD(T)/e1{T,Q}Z	SDT/e1{T,Q}Z	SDT(Q)/e1{T,Q}Z	SD(T)/e2{D,T}Z	SDT/e2{D,T}Z	SDT(Q)/e2{D,T}Z	SD(T)/e2{T,Q}Z	SDT/e2{T,Q}Z	SDT(Q)/e2{T,Q}Z	SD(T)/e3{D,T}Z	SDT/e3{D,T}Z	SDT(Q)/e3{D,T}Z	SD(T)/e3{T,Q}Z	SDT/e3{T,Q}Z	SDT(Q)/e3{T,Q}Z
nh2	0.4436	0.0049	0.0818	0.0813	0.0798	0.0612	0.0514	0.0509	0.0339	0.0224	0.0215	0.0534	0.0397	0.0396	0.0154	0.0027	0.0016	0.0515	0.0371	0.0370	0.0158	0.0027	0.0016	0.0512	0.0358	0.0359	0.0110	0.0020	0.0032
no	0.6905	0.0061	0.1795	0.1824	0.1682	0.1212	0.0944	0.0840	0.0751	0.0418	0.0322	0.1034	0.0640	0.0552	0.0494	0.0114	0.0024	0.1053	0.0636	0.0548	0.0499	0.0105	0.0013	0.1055	0.0606	0.0526	0.0443	0.0052	0.0037
oh	0.2107	0.0018	0.0232	0.0236	0.0221	0.0236	0.0215	0.0191	0.0131	0.0108	0.0078	0.0242	0.0210	0.0183	0.0065	0.0040	0.0005	0.0250	0.0216	0.0189	0.0066	0.0041	0.0007	0.0251	0.0215	0.0186	0.0050	0.0025	0.0012
sih	0.0489	0.0006	0.1019	0.0991	0.1031	0.0175	0.0042	0.0047	0.0147	0.0087	0.0019	0.0169	0.0466	0.0356	0.0131	0.0116	0.0003	0.0289	0.0600	0.0490	0.0131	0.0120	0.0003	0.0304	0.0636	0.0517	0.0127	0.0122	0.0000
ch2-trip	0.8625	0.0133	0.4072	0.4076	0.4096	0.1182	0.1167	0.1204	0.0509	0.0487	0.0528	0.0035	0.0058	0.0014	0.0021	0.0006	0.0038	0.0507	0.0531	0.0487	0.0033	0.0004	0.0048	0.0568	0.0595	0.0547	0.0101	0.0130	0.0085
nh	0.1737	0.0015	0.0098	0.0100	0.0093	0.0215	0.0170	0.0168	0.0127	0.0075	0.0069	0.0268	0.0204	0.0203	0.0070	0.0013	0.0005	0.0292	0.0225	0.0224	0.0071	0.0012	0.0005	0.0295	0.0223	0.0223	0.0057	0.0002	0.0010
o2	0.4139	0.0018	0.0614	0.0598	0.0524	0.0697	0.0347	0.0360	0.0515	0.0095	0.0125	0.0812	0.0321	0.0371	0.0441	0.0029	0.0012	0.0963	0.0446	0.0496	0.0442	0.0044	0.0005	0.0982	0.0429	0.0495	0.0433	0.0050	0.0006
		MAX	0.7185	0.7174	0.7222	0.3118	0.2543	0.2354	0.1838	0.1197	0.1017	0.1474	0.1220	0.1198	0.0938	0.0249	0.0076	0.1456	0.1544	0.1522	0.0960	0.0255	0.0081	0.1497	0.1600	0.1573	0.0717	0.0218	0.0156
		MAD	0.2312	0.2298	0.2269	0.0961	0.0807	0.0791	0.0531	0.0353	0.0336	0.0591	0.0424	0.0384	0.0247	0.0063	0.0024	0.0619	0.0469	0.0427	0.0253	0.0064	0.0027	0.0626	0.0468	0.0436	0.0211	0.0064	0.0051
		RMS	0.3166	0.3136	0.3096	0.1276	0.1100	0.1068	0.0695	0.0482	0.0452	0.0730	0.0522	0.0482	0.0342	0.0089	0.0033	0.0722	0.0577	0.0542	0.0349	0.0090	0.0036	0.0730	0.0593	0.0559	0.0283	0.0086	0.0069
		SD	0.2208	0.2178	0.2150	0.0856	0.0763	0.0733	0.0458	0.0335	0.0309	0.0438	0.0311	0.0297	0.0241	0.0063	0.0022	0.0380	0.0344	0.0341	0.0245	0.0065	0.0024	0.0383	0.0372	0.0358	0.0192	0.0059	0.0047

Table S13. Differences between absolute deviations obtained at given levels of theory in kcal mol⁻¹. The geometries were optimized as indicated in the header of Table S12. Reference values are computed as the mean of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values. Positive values are highlighted in red. Maximum (MAX), mean (MAD), root mean square (RMS), and standard deviation (SD) are provided at the bottom of the Table.

System	$\frac{\text{SDT/DZ}}{\text{SD(T)/TZ}}$	$\frac{\text{SDT(Q)/DZ}}{\text{SD(T)/TZ}}$	$\frac{\text{SDT/TZ}}{\text{SD(T)/QZ}}$	$\frac{\text{SDT(Q)/TZ}}{\text{SD(T)/QZ}}$	$\frac{\text{SDT/e1\{D,T\}Z}}{\text{SD(T)/e1\{T,Q\}Z}}$	$\frac{\text{SDT(Q)/e1\{D,T\}Z}}{\text{SD(T)/e1\{T,Q\}Z}}$	$\frac{\text{SDT/e2\{D,T\}Z}}{\text{SD(T)/e2\{T,Q\}Z}}$	$\frac{\text{SDT(Q)/e2\{D,T\}Z}}{\text{SD(T)/e2\{T,Q\}Z}}$	$\frac{\text{SDT/e3\{D,T\}Z}}{\text{SD(T)/e3\{T,Q\}Z}}$	$\frac{\text{SDT(Q)/e3\{D,T\}Z}}{\text{SD(T)/e3\{T,Q\}Z}}$
alh	0.1105	0.1423	-0.0007	0.0407	0.0064	-0.0067	0.0268	0.0142	0.0361	0.0118
bf	0.2486	0.2596	0.0906	0.1023	0.0562	0.0691	0.0207	0.0343	0.0342	0.0368
bh	0.0945	0.1086	0.0081	0.0246	-0.0072	0.0036	0.0078	0.0189	0.0146	0.0177
bh3	0.5313	0.5385	0.1029	0.1136	0.0379	0.0317	0.1230	0.1203	0.1231	0.1099
ch2-sing	0.0862	0.1194	0.0010	0.0387	-0.0242	0.0165	-0.0408	0.0008	-0.0371	-0.0030
co	0.3204	0.3352	0.0971	0.1180	0.0419	0.0670	0.0026	0.0289	0.0159	0.0383
f2	0.0255	0.0463	-0.0227	0.0082	-0.0410	0.0043	-0.0266	0.0200	-0.0321	0.0153
h2o	0.0355	0.0379	0.0231	0.0256	0.0261	0.0288	0.0212	0.0242	0.0251	0.0278
h2s	0.1677	0.1646	0.0183	0.0119	0.1179	0.1164	0.1507	0.1476	0.1515	0.1569
hcl	0.0821	0.0862	-0.0014	0.0072	0.0419	0.0429	0.0563	0.0577	0.0565	0.0582
hf	0.0178	0.0146	0.0118	0.0058	0.0121	0.0047	0.0100	0.0025	0.0114	0.0036
n2	0.2590	0.2950	0.0570	0.1119	0.0037	0.0693	-0.0214	0.0463	-0.0140	0.0339
nh3	0.0952	0.1077	0.0379	0.0554	0.0295	0.0501	0.0136	0.0348	0.0202	0.0307
cf	0.0445	0.0489	0.0188	0.0216	0.0167	0.0194	0.0132	0.0164	0.0162	0.0186
ch	0.0234	0.0351	0.0014	0.0150	-0.0040	0.0108	-0.0083	0.0068	-0.0073	0.0042
ch3	0.3213	0.3291	0.0758	0.0879	-0.0027	0.0116	0.0350	0.0399	0.0479	0.0327
cn	0.3869	0.4205	0.0705	0.1156	-0.0209	0.0312	-0.0823	-0.0223	-0.0697	0.0125
hs	0.0624	0.0614	0.0129	0.0086	0.0606	0.0591	0.0750	0.0726	0.0747	0.0773
nh2	0.0201	0.0283	0.0176	0.0285	0.0243	0.0369	0.0212	0.0343	0.0248	0.0339
no	0.0611	0.0739	0.0193	0.0422	0.0146	0.0438	0.0137	0.0444	0.0163	0.0474
oh	0.0000	0.0006	0.0084	0.0084	0.0146	0.0143	0.0150	0.0148	0.0165	0.0162
sih	0.0816	0.0989	-0.0105	-0.0040	0.0335	0.0240	0.0469	0.0371	0.0509	0.0395

System	$\frac{SDT/DZ}{-SD(T)/TZ}$	$\frac{SDT(Q)/DZ}{-SDT/TZ}$	$\frac{SDT/TZ}{-SD(T)/QZ}$	$\frac{SDT(Q)/TZ}{-SDT/QZ}$	$\frac{SDT/e1\{D,T\}Z}{-SD(T)/e1\{T,Q\}Z}$	$\frac{SDT(Q)/e1\{D,T\}Z}{-SDT/e1\{T,Q\}Z}$	$\frac{SDT/e2\{D,T\}Z}{-SD(T)/e2\{T,Q\}Z}$	$\frac{SDT(Q)/e2\{D,T\}Z}{-SDT/e2\{T,Q\}Z}$	$\frac{SDT/e3\{D,T\}Z}{-SD(T)/e3\{T,Q\}Z}$	$\frac{SDT(Q)/e3\{D,T\}Z}{-SDT/e3\{T,Q\}Z}$
ch2-trip	0.2895	0.2930	0.0658	0.0717	0.0037	0.0008	0.0498	0.0482	0.0493	0.0418
nh	-0.0115	-0.0077	0.0044	0.0093	0.0133	0.0190	0.0153	0.0212	0.0166	0.0221
o2	-0.0099	0.0177	-0.0168	0.0264	-0.0120	0.0342	0.0004	0.0452	-0.0004	0.0445
MAX	0.4056	0.4679	0.0705	0.1156	0.0282	0.0949	0.0584	0.1267	0.0883	0.1355
MAD	0.1337	0.1462	0.0276	0.0438	0.0177	0.0321	0.0215	0.0364	0.0256	0.0371
RMS	0.1861	0.1996	0.0405	0.0587	0.0180	0.0394	0.0229	0.0452	0.0310	0.0473
SD	0.1322	0.1387	0.0305	0.0398	0.0070	0.0234	0.0099	0.0275	0.0180	0.0299

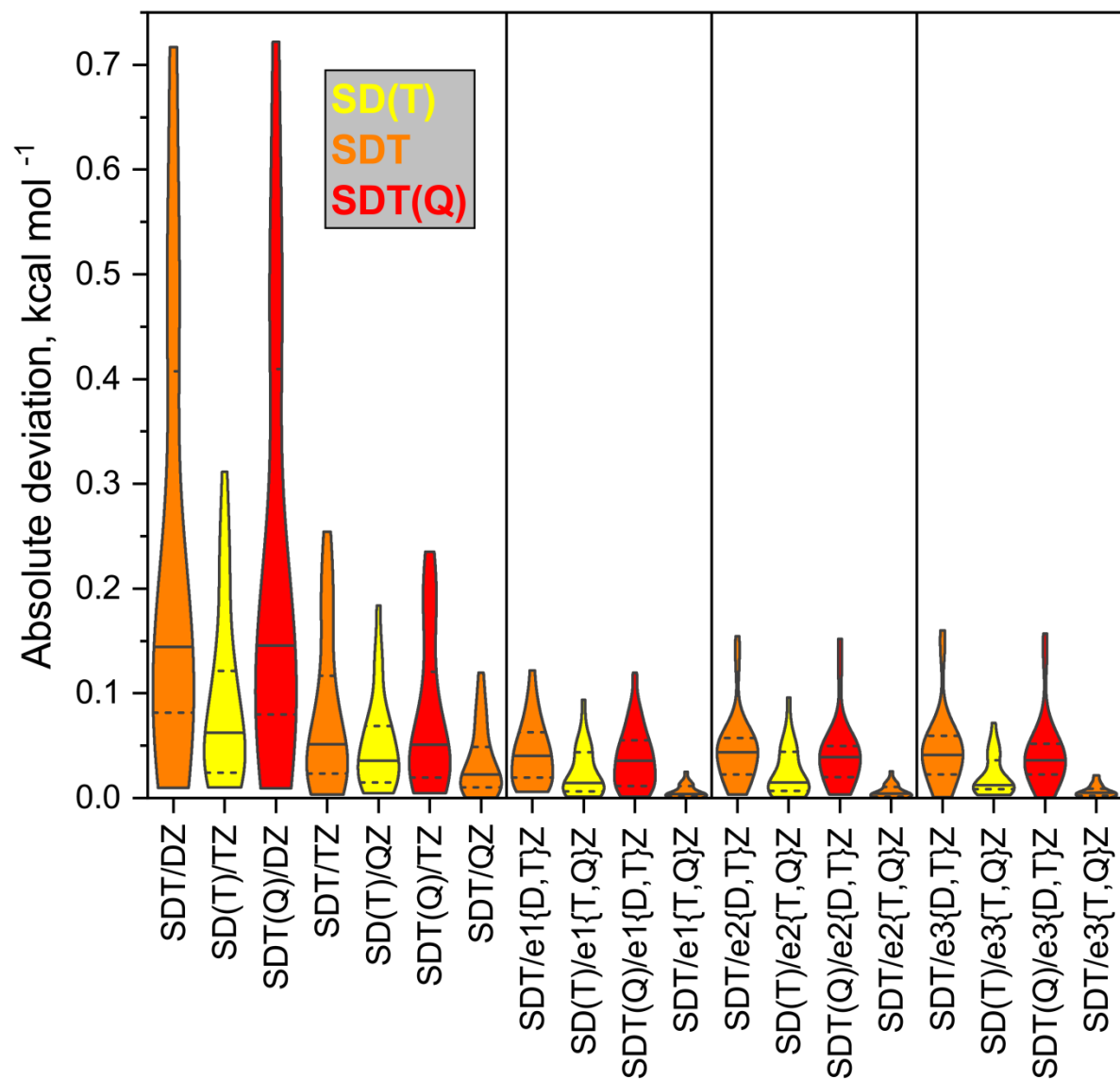


Figure S14. Violin plots of the absolute deviations obtained at a given level of theory. The geometries were optimized as indicated in the header of Table S12. Reference values are computed as the mean of $\text{SDT(Q)/eN}\{\text{T,Q}\}\text{Z}$ ($N = 1 - 3$) values. The median (solid), 25th, and 75th percentiles (dash) are shown. The highest point of a plot represents the maximum deviation.

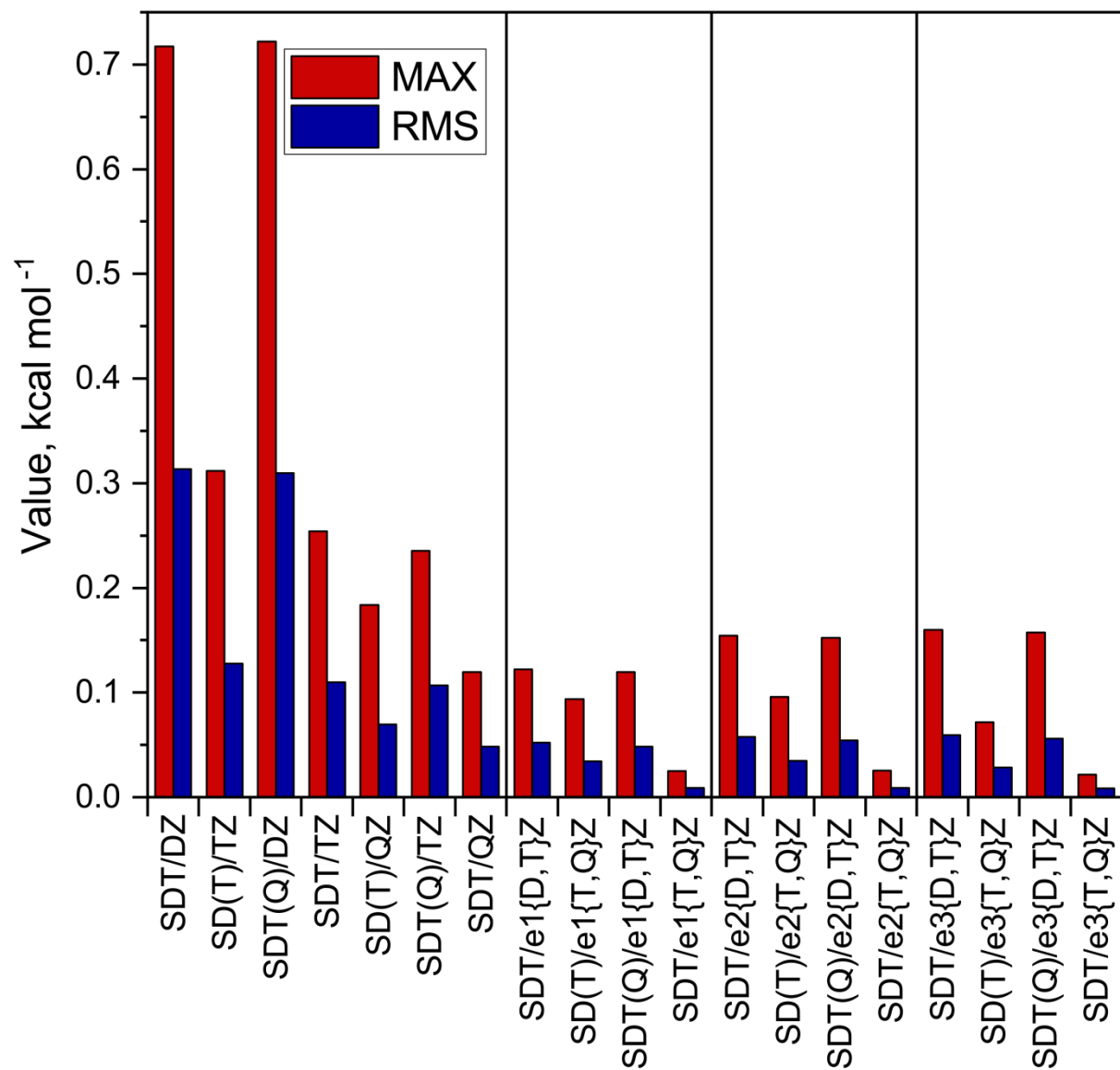


Figure S15. Maximum (MAX) and root mean square (RMS) values for the absolute deviations obtained at a given level of theory. The geometries were optimized as indicated in the header of Table S12. Reference values are computed as the mean of SDT(Q)/eN{T,Q}Z (N = 1 – 3) values.

Geometry Data

Table S14. Bond lengths for diatomic systems optimized using FC-SD(T)/nZ and FC-SDT/nZ methods, in Å.

System	Multiplicity	Basis set	$l_{\text{FC-SD(T)}}$	$l_{\text{FC-SDT}}$	Difference
alh	1	DZ	1.65404	1.65461	0.00057
		TZ	1.64984	1.65029	0.00045
		QZ	1.64925	1.64925	0
co	1	DZ	1.14248	1.14263	0.00015
		TZ	1.13333	1.13320	0.00013
		QZ	1.13094	1.13075	0.00019
f2	1	DZ	1.45577	1.45577	0
		TZ	1.41448	1.41418	0.0003
		QZ	1.41259	1.41216	0.00043
hcl	1	DZ	1.28485	1.28497	0.00012
		TZ	1.27369	1.27369	0
		QZ	1.27514	1.27514	0
cf	2	DZ	1.29146	1.29249	0.00103
		TZ	1.27587	1.27648	0.00061
		QZ	1.27443	1.27494	0.00051
hs	2	DZ	1.35357	1.35382	0.00025
		TZ	1.34113	1.34132	0.00019
		QZ	1.34151	1.34170	0.00019
		5Z	1.34163	1.34181	0.00018
no	2	DZ	1.15990	1.16462	0.00472
		TZ	1.15167	1.15499	0.00332
		QZ	1.14960	1.15245	0.00285
sih	2	DZ	1.53392	1.53439	0.00047
		TZ	1.52253	1.52290	0.00037
		QZ	1.52150	1.52184	0.00034
		5Z	1.52166	1.52199	0.00033
bn3pi	3	DZ	1.34281	1.34603	0.00322
		TZ	1.33125	1.33346	0.00221
		QZ	1.32747	1.32940	0.00193
nh	3	DZ	1.05548	1.05575	0.00027
		TZ	1.03858	1.03880	0.00022
		QZ	1.03724	1.03747	0.00023
		5Z	1.03681	1.03702	0.00021

Table S15. Bond lengths for diatomic systems optimized using FC-SD(T)/nZ and CV-SD(T)/nZ methods, in Å.

System	Multiplicity	Basis set	$l_{\text{FC-SD(T)}}$	$l_{\text{CV-SD(T)}}$	Difference
alh	1	DZ	1.65404	1.65560	0.00156
		TZ	1.64984	1.64618	0.00366
		QZ	1.64925	1.64465	0.00460
bf	1	DZ	1.29297	1.29176	0.00121
		TZ	1.26822	1.26505	0.00317
		QZ	1.26658	1.26272	0.00386
bh	1	DZ	1.25398	1.25325	0.00073
		TZ	1.23448	1.23172	0.00276
		QZ	1.23305	1.22988	0.00317
co	1	DZ	1.14248	1.14175	0.00073
		TZ	1.13333	1.13136	0.00197
		QZ	1.13094	1.12860	0.00234
f2	1	DZ	1.45577	1.45497	0.00080
		TZ	1.41448	1.41326	0.00122
		QZ	1.41259	1.41121	0.00138
hcl	1	DZ	1.28485	1.28448	0.00037
		TZ	1.27369	1.27226	0.00143
		QZ	1.27514	1.27334	0.00180
hf	1	DZ	0.91979	0.91945	0.00034
		TZ	0.91708	0.91658	0.00050
		QZ	0.91636	0.91579	0.00057
n2	1	DZ	1.11718	1.11658	0.00060
		TZ	1.10164	1.09994	0.00170
		QZ	1.09996	1.09794	0.00202
cf	2	DZ	1.29146	1.29033	0.00113
		TZ	1.27587	1.27341	0.00246
		QZ	1.27443	1.27152	0.00291
ch	2	DZ	1.14247	1.14173	0.00074
		TZ	1.12191	1.12027	0.00164
		QZ	1.12024	1.11835	0.00189

System	Multiplicity	Basis set	I_{FC-SD(T)}	I_{CV-SD(T)}	Difference
cn	2	DZ	1.18812	1.18735	0.00077
		TZ	1.17192	1.16971	0.00221
		QZ	1.16969	1.16710	0.00259
hs	2	DZ	1.35357	1.35340	0.00017
		TZ	1.34113	1.33935	0.00178
		QZ	1.34151	1.33929	0.00222
no	2	DZ	1.15990	1.15928	0.00062
		TZ	1.15167	1.15028	0.00139
		QZ	1.14960	1.14796	0.00164
oh	2	DZ	0.97937	0.97888	0.00049
		TZ	0.97066	0.96994	0.00072
		QZ	0.96972	0.96889	0.00083
sih	2	DZ	1.53392	1.53477	0.00085
		TZ	1.52253	1.51973	0.00280
		QZ	1.52150	1.51804	0.00346
nh	3	DZ	1.05548	1.05483	0.00065
		TZ	1.03858	1.03751	0.00107
		QZ	1.03724	1.03602	0.00122
o2	3	DZ	1.21574	1.21484	0.00090
		TZ	1.21143	1.20973	0.00170
		QZ	1.20758	1.20567	0.00191

Cartesian Coordinates of Optimized Structures

The data below are given in multiple XYZ-file format: the first line is the number of atoms (N), the second line is a comment presenting the system and level of theory for geometry optimization, and the following N lines contain atomic cartesian coordinates. Multiple structures are placed directly end-to-end.

```
2
alh FC-CCSD(T)/cc-pwCVDZ
  Al  0.0000000000000000    0.0000000000000000    -0.06146191349881
  H   0.0000000000000000    0.0000000000000000     1.59257872219881
2
alh FC-CCSD(T)/cc-pwCVQZ
  Al  0.0000000000000000    0.0000000000000000    -0.05906471174294
  H   0.0000000000000000    0.0000000000000000     1.59018152044294
2
alh FC-CCSD(T)/cc-pwCVTZ
  Al  0.0000000000000000    0.0000000000000000    -0.05936005525947
  H   0.0000000000000000    0.0000000000000000     1.59047686395947
2
alh CV-CCSD(T)/cc-pwCVDZ
  Al  0.0000000000000000    0.0000000000000000    -0.06224390942335
  H   0.0000000000000000    0.0000000000000000     1.59336071812335
2
alh CV-CCSD(T)/cc-pwCVQZ
  Al  0.0000000000000000    0.0000000000000000    -0.05676810369397
  H   0.0000000000000000    0.0000000000000000     1.58788491239397
2
alh CV-CCSD(T)/cc-pwCVTZ
  Al  0.0000000000000000    0.0000000000000000    -0.05753390679309
  H   0.0000000000000000    0.0000000000000000     1.58865071549309
2
bf FC-CCSD(T)/cc-pwCVDZ
  F   0.0000000000000000    0.0000000000000000    -0.47245947473382
  B   0.0000000000000000    0.0000000000000000     0.82050890613382
2
bf FC-CCSD(T)/cc-pwCVQZ
  F   0.0000000000000000    0.0000000000000000    -0.45926344550911
  B   0.0000000000000000    0.0000000000000000     0.80731287690911
2
bf FC-CCSD(T)/cc-pwCVTZ
  F   0.0000000000000000    0.0000000000000000    -0.46008381848103
  B   0.0000000000000000    0.0000000000000000     0.80813324988103
2
bf CV-CCSD(T)/cc-pwCVDZ
```

F	0.0000000000000000	0.0000000000000000	-0.47185345640309
B	0.0000000000000000	0.0000000000000000	0.81990288780309
2			
bf CV-CCSD(T)/cc-pwCVQZ			
F	0.0000000000000000	0.0000000000000000	-0.45733700734489
B	0.0000000000000000	0.0000000000000000	0.80538643874489
2			
bf CV-CCSD(T)/cc-pwCVTZ			
F	0.0000000000000000	0.0000000000000000	-0.45850225031811
B	0.0000000000000000	0.0000000000000000	0.80655168171811
2			
bh FC-CCSD(T)/cc-pwCVDZ			
B	0.0000000000000000	0.0000000000000000	-0.11583293535711
H	0.0000000000000000	0.0000000000000000	1.13815195775711
2			
bh FC-CCSD(T)/cc-pwCVQZ			
B	0.0000000000000000	0.0000000000000000	-0.10536544615304
H	0.0000000000000000	0.0000000000000000	1.12768446855304
2			
bh FC-CCSD(T)/cc-pwCVTZ			
B	0.0000000000000000	0.0000000000000000	-0.10607821877459
H	0.0000000000000000	0.0000000000000000	1.12839724117459
2			
bh CV-CCSD(T)/cc-pwCVDZ			
B	0.0000000000000000	0.0000000000000000	-0.11546299488672
H	0.0000000000000000	0.0000000000000000	1.13778201728672
2			
bh CV-CCSD(T)/cc-pwCVQZ			
B	0.0000000000000000	0.0000000000000000	-0.10378177997868
H	0.0000000000000000	0.0000000000000000	1.12610080237868
2			
bh CV-CCSD(T)/cc-pwCVTZ			
B	0.0000000000000000	0.0000000000000000	-0.10469805635353
H	0.0000000000000000	0.0000000000000000	1.12701707875353
4			
bh3 FC-CCSD(T)/cc-pwCVDZ			
B	-0.00000366427346	-0.00000000000199	0.00000000215549
H	1.20599805442900	0.00000000000733	-0.00000000071849
H	-0.60299719508354	-1.04442862693567	-0.00000000071850
H	-0.60299719507200	1.04442862693033	-0.00000000071850
4			
bh3 FC-CCSD(T)/cc-pwCVQZ			
B	-0.00000334872482	-0.00000000000383	0.00000000038431
H	1.18968328350717	0.00000000000829	-0.00000000012810

H	-0.59483996739726	-1.03029897327639	-0.00000000012810
H	-0.59483996738510	1.03029897327192	-0.00000000012810
4			
bh3 FC-CCSD(T)/cc-pwCVTZ			
B	-0.00000334204855	-0.00000000000067	0.00000000008718
H	1.19052165463050	0.00000000000235	-0.0000000002906
H	-0.59525915629282	-1.03102501195480	-0.0000000002906
H	-0.59525915628914	1.03102501195312	-0.0000000002906
4			
bh3 CV-CCSD(T)/cc-pwCVDZ			
B	-0.00000366433466	-0.00000000000230	0.00000000251685
H	1.20542149583609	0.00000000000070	-0.00000000083894
H	-0.60270891575066	-1.04392931577895	-0.00000000083895
H	-0.60270891575077	1.04392931578054	-0.00000000083895
4			
bh3 CV-CCSD(T)/cc-pwCVQZ			
B	-0.00000334870035	-0.00000000001568	0.00000000084409
H	1.18722074954800	0.00000000002646	-0.00000000028136
H	-0.59360870044221	-1.02816635277820	-0.00000000028136
H	-0.59360870040544	1.02816635276742	-0.00000000028136
4			
bh3 CV-CCSD(T)/cc-pwCVTZ			
B	-0.00000334405155	0.00000000000056	0.00000000099832
H	1.18840584274196	0.00000000000184	-0.00000000033277
H	-0.59420124934696	-1.02919266541192	-0.00000000033278
H	-0.59420124934345	1.02919266540952	-0.00000000033278
2			
cf FC-CCSD(T)/cc-pwCVDZ			
C	0.00000000000000	0.00000000000000	-0.78930287112333
F	0.00000000000000	0.00000000000000	0.50215321862333
2			
cf FC-CCSD(T)/cc-pwCVQZ			
C	0.00000000000000	0.00000000000000	-0.78078876022010
F	0.00000000000000	0.00000000000000	0.49363910772010
2			
cf FC-CCSD(T)/cc-pwCVTZ			
C	0.00000000000000	0.00000000000000	-0.78150734554360
F	0.00000000000000	0.00000000000000	0.49435769304360
2			
cf CV-CCSD(T)/cc-pwCVDZ			
C	0.00000000000000	0.00000000000000	-0.78874081028933
F	0.00000000000000	0.00000000000000	0.50159115778933
2			
cf CV-CCSD(T)/cc-pwCVQZ			

C	0.0000000000000000	0.0000000000000000	-0.77933415798447
F	0.0000000000000000	0.0000000000000000	0.49218450548447
2			
cf CV-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.78027989841505
F	0.0000000000000000	0.0000000000000000	0.49313024591505
2			
ch FC-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	0.0000000000000000	-0.09809531062832
H	0.0000000000000000	0.0000000000000000	1.04437418182832
2			
ch FC-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.0000000000000000	-0.08697876087016
H	0.0000000000000000	0.0000000000000000	1.03325763207016
2			
ch FC-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.08781716738135
H	0.0000000000000000	0.0000000000000000	1.03409603858135
2			
ch CV-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	0.0000000000000000	-0.09772780410847
H	0.0000000000000000	0.0000000000000000	1.04400667530847
2			
ch CV-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.0000000000000000	-0.08603362863220
H	0.0000000000000000	0.0000000000000000	1.03231249983220
2			
ch CV-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.08699529541127
H	0.0000000000000000	0.0000000000000000	1.03327416661127
3			
ch2-sing FC-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	-0.000000000000426	-0.11633714036968
H	0.0000000000000000	0.86794234511250	0.60485472013665
H	0.0000000000000000	-0.86794234510824	0.60485472013303
3			
ch2-sing FC-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.000000000000895	-0.10112507836720
H	0.0000000000000000	0.86094357227052	0.59724868913000
H	0.0000000000000000	-0.86094357227947	0.59724868913721
3			
ch2-sing FC-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.000000000000298	-0.10301459124230
H	0.0000000000000000	0.86039471918268	0.59819344556990

H	0.0000000000000000	-0.86039471918566	0.59819344557240
3	ch2-sing CV-CCSD(T)/cc-pwCVDZ		
C	0.0000000000000000	-0.000000000000498	-0.11571269169942
H	0.0000000000000000	0.86769807925977	0.60454249580181
H	0.0000000000000000	-0.86769807925479	0.60454249579761
3	ch2-sing CV-CCSD(T)/cc-pwCVQZ		
C	0.0000000000000000	0.000000000000384	-0.09961909023104
H	0.0000000000000000	0.86029316222501	0.59649569506397
H	0.0000000000000000	-0.86029316222884	0.59649569506707
3	ch2-sing CV-CCSD(T)/cc-pwCVTZ		
C	0.0000000000000000	0.000000000000194	-0.10167999305833
H	0.0000000000000000	0.85985138723209	0.59752614647839
H	0.0000000000000000	-0.85985138723403	0.59752614647994
3	ch2-trip FC-CCSD(T)/cc-pwCVDZ		
C	0.0000000000000000	-0.000000000000292	-0.07374721900459
H	0.0000000000000000	1.00103013072673	0.36894328900284
H	0.0000000000000000	-1.00103013072381	0.36894328900175
3	ch2-trip FC-CCSD(T)/cc-pwCVQZ		
C	0.0000000000000000	-0.000000000001577	-0.06118323269066
H	0.0000000000000000	0.99023955877414	0.36266129584870
H	0.0000000000000000	-0.99023955875837	0.36266129584196
3	ch2-trip FC-CCSD(T)/cc-pwCVTZ		
C	0.0000000000000000	0.000000000000736	-0.06236430612219
H	0.0000000000000000	0.99034544920794	0.36325183255951
H	0.0000000000000000	-0.99034544921530	0.36325183256267
3	ch2-trip CV-CCSD(T)/cc-pwCVDZ		
C	0.0000000000000000	-0.000000000000403	-0.07309812018879
H	0.0000000000000000	1.00079141096506	0.36861873959528
H	0.0000000000000000	-1.00079141096103	0.36861873959351
3	ch2-trip CV-CCSD(T)/cc-pwCVQZ		
C	0.0000000000000000	-0.000000000001142	-0.05989610687288
H	0.0000000000000000	0.98939411327683	0.36201773293888
H	0.0000000000000000	-0.98939411326541	0.36201773293399
3	ch2-trip CV-CCSD(T)/cc-pwCVTZ		
C	0.0000000000000000	-0.000000000001114	-0.06120451634709

H	0.0000000000000000	0.98964716425939	0.36267193767594
H	0.0000000000000000	-0.98964716424824	0.36267193767115
4			
ch3	FC-CCSD(T)/cc-pwCVDZ		
C	-0.00000430033762	0.00000000004798	0.00000000028297
H	1.09369511060876	-0.00000000003495	-0.00000000009432
H	-0.54684540516916	-0.94717192084107	-0.00000000009432
H	-0.54684540520199	0.94717192082803	-0.00000000009432
4			
ch3	FC-CCSD(T)/cc-pwCVQZ		
C	-0.00000340416802	0.00000000002461	0.00000000021307
H	1.07761108331161	0.00000000001733	-0.00000000007102
H	-0.53880383964391	-0.93324133430089	-0.00000000007102
H	-0.53880383959969	0.93324133425895	-0.00000000007102
4			
ch3	FC-CCSD(T)/cc-pwCVTZ		
C	-0.00000340898861	-0.00000000002072	0.00000000018076
H	1.07829472524295	0.00000000004332	-0.00000000006025
H	-0.53914565820870	-0.93383338750084	-0.00000000006025
H	-0.53914565814564	0.93383338747824	-0.00000000006025
4			
ch3	CV-CCSD(T)/cc-pwCVDZ		
C	-0.00000729088936	0.00000000002211	0.00000000031781
H	1.09312453719766	-0.00000000001248	-0.00000000010594
H	-0.54655862319972	-0.94668333537391	-0.00000000010594
H	-0.54655862320858	0.94668333536428	-0.00000000010594
4			
ch3	CV-CCSD(T)/cc-pwCVQZ		
C	-0.00000340272298	-0.00000000003071	-0.00000000008598
H	1.07617237325152	0.00000000003379	0.00000000002866
H	-0.53808448533467	-0.93199536934168	0.00000000002866
H	-0.53808448529388	0.93199536933861	0.00000000002866
4			
ch3	CV-CCSD(T)/cc-pwCVTZ		
C	-0.00000340862495	0.00000000004601	-0.00000000038261
H	1.07705680682805	-0.00000000003836	0.00000000012753
H	-0.53852669913161	-0.93276131524801	0.00000000012754
H	-0.53852669917149	0.93276131524036	0.00000000012754
2			
cn	FC-CCSD(T)/cc-pwCVDZ		
C	0.0000000000000000	0.0000000000000000	-0.63907023857934
N	0.0000000000000000	0.0000000000000000	0.54904778757934
2			
cn	FC-CCSD(T)/cc-pwCVQZ		

C	0.0000000000000000	0.0000000000000000	-0.62985746689941
N	0.0000000000000000	0.0000000000000000	0.53983501589941
2			
cn FC-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.63097267446294
N	0.0000000000000000	0.0000000000000000	0.54095022346294
2			
cn CV-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	0.0000000000000000	-0.63868861453772
N	0.0000000000000000	0.0000000000000000	0.54866616353772
2			
cn CV-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.0000000000000000	-0.62856135778943
N	0.0000000000000000	0.0000000000000000	0.53853890678943
2			
cn CV-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.62986707781360
N	0.0000000000000000	0.0000000000000000	0.53984462681360
2			
co FC-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	0.0000000000000000	-0.65173335913075
O	0.0000000000000000	0.0000000000000000	0.49074687473075
2			
co FC-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.0000000000000000	-0.64596142695238
O	0.0000000000000000	0.0000000000000000	0.48497494255238
2			
co FC-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.64715761095068
O	0.0000000000000000	0.0000000000000000	0.48617112655068
2			
co CV-CCSD(T)/cc-pwCVDZ			
C	0.0000000000000000	0.0000000000000000	-0.65136848604265
O	0.0000000000000000	0.0000000000000000	0.49038200164265
2			
co CV-CCSD(T)/cc-pwCVQZ			
C	0.0000000000000000	0.0000000000000000	-0.64479529581179
O	0.0000000000000000	0.0000000000000000	0.48380881141179
2			
co CV-CCSD(T)/cc-pwCVTZ			
C	0.0000000000000000	0.0000000000000000	-0.64617266797506
O	0.0000000000000000	0.0000000000000000	0.48518618357506
2			
f2 FC-CCSD(T)/cc-pwCVDZ			

F	0.0000000000000000	0.0000000000000000	-0.72788598451977
F	0.0000000000000000	0.0000000000000000	0.72788598451977
2			
f2	FC-CCSD(T)/cc-pwCVQZ		
F	0.0000000000000000	0.0000000000000000	-0.70629713754918
F	0.0000000000000000	0.0000000000000000	0.70629713754918
2			
f2	FC-CCSD(T)/cc-pwCVTZ		
F	0.0000000000000000	0.0000000000000000	-0.70724206541794
F	0.0000000000000000	0.0000000000000000	0.70724206541794
2			
f2	CV-CCSD(T)/cc-pwCVDZ		
F	0.0000000000000000	0.0000000000000000	-0.72748499803160
F	0.0000000000000000	0.0000000000000000	0.72748499803160
2			
f2	CV-CCSD(T)/cc-pwCVQZ		
F	0.0000000000000000	0.0000000000000000	-0.70560675618986
F	0.0000000000000000	0.0000000000000000	0.70560675618986
2			
f2	CV-CCSD(T)/cc-pwCVTZ		
F	0.0000000000000000	0.0000000000000000	-0.70663142304156
F	0.0000000000000000	0.0000000000000000	0.70663142304156
3			
h2o	FC-CCSD(T)/cc-pwCVDZ		
O	0.0000000000000000	-0.000000000000554	-0.08007605601922
H	0.0000000000000000	0.75029964774694	0.52859183416192
H	0.0000000000000000	-0.75029964774140	0.52859183415730
3			
h2o	FC-CCSD(T)/cc-pwCVQZ		
O	0.0000000000000000	0.00000000001925	-0.06699573847930
H	0.0000000000000000	0.75548199922188	0.52205167538214
H	0.0000000000000000	-0.75548199924113	0.52205167539716
3			
h2o	FC-CCSD(T)/cc-pwCVTZ		
O	0.0000000000000000	0.00000000000939	-0.06965969801190
H	0.0000000000000000	0.75362575482512	0.52338365515225
H	0.0000000000000000	-0.75362575483451	0.52338365515965
3			
h2o	CV-CCSD(T)/cc-pwCVDZ		
O	0.0000000000000000	-0.00000000000220	-0.07955554641082
H	0.0000000000000000	0.75025947939629	0.52833157935621
H	0.0000000000000000	-0.75025947939410	0.52833157935461
3			
h2o	CV-CCSD(T)/cc-pwCVQZ		

O	0.0000000000000000	0.00000000001377	-0.06611159828956
H	0.0000000000000000	0.75539860219886	0.52160960528943
H	0.0000000000000000	-0.75539860221263	0.52160960530014
3			
h2o CV-CCSD(T)/cc-pwCVTZ			
O	0.0000000000000000	0.00000000000045	-0.06886304874201
H	0.0000000000000000	0.75357572032949	0.52298533052086
H	0.0000000000000000	-0.75357572032994	0.52298533052115
3			
h2s FC-CCSD(T)/cc-pwCVDZ			
S	0.0000000000000000	0.00000000001295	-0.05991153744251
H	0.0000000000000000	0.97151388672206	0.87401003881501
H	0.0000000000000000	-0.97151388673501	0.87401003882749
3			
h2s FC-CCSD(T)/cc-pwCVQZ			
S	0.0000000000000000	0.00000000007877	-0.05467208400658
H	0.0000000000000000	0.96456789552453	0.87139031206548
H	0.0000000000000000	-0.96456789560329	0.87139031214110
3			
h2s FC-CCSD(T)/cc-pwCVTZ			
S	0.0000000000000000	0.00000000002510	-0.05463017282005
H	0.0000000000000000	0.96364544195756	0.87136935649793
H	0.0000000000000000	-0.96364544198266	0.87136935652211
3			
h2s CV-CCSD(T)/cc-pwCVDZ			
S	0.0000000000000000	0.00000000001027	-0.06011120275078
H	0.0000000000000000	0.97082393162312	0.87410987147051
H	0.0000000000000000	-0.97082393163338	0.87410987148027
3			
h2s CV-CCSD(T)/cc-pwCVQZ			
S	0.0000000000000000	-0.00000000010085	-0.05377528806361
H	0.0000000000000000	0.96266201575315	0.87094191418024
H	0.0000000000000000	-0.96266201565230	0.87094191408337
3			
h2s CV-CCSD(T)/cc-pwCVTZ			
S	0.0000000000000000	-0.00000000003957	-0.05397009224991
H	0.0000000000000000	0.96199598695877	0.87103931624397
H	0.0000000000000000	-0.96199598691920	0.87103931620593
2			
hcl FC-CCSD(T)/cc-pwCVDZ			
Cl	0.0000000000000000	0.00000000000000	-0.03970503817190
H	0.0000000000000000	0.00000000000000	1.24514778017190
2			
hcl FC-CCSD(T)/cc-pwCVQZ			

C1	0.0000000000000000	0.0000000000000000	-0.03484957649777
H	0.0000000000000000	0.0000000000000000	1.24029231849777
2			
hcl	FC-CCSD(T)/cc-pwCVTZ		
C1	0.0000000000000000	0.0000000000000000	-0.03412427511101
H	0.0000000000000000	0.0000000000000000	1.23956701711101
2			
hcl	CV-CCSD(T)/cc-pwCVDZ		
C1	0.0000000000000000	0.0000000000000000	-0.03951963742323
H	0.0000000000000000	0.0000000000000000	1.24496237942323
2			
hcl	CV-CCSD(T)/cc-pwCVQZ		
C1	0.0000000000000000	0.0000000000000000	-0.03394782855197
H	0.0000000000000000	0.0000000000000000	1.23939057055197
2			
hcl	CV-CCSD(T)/cc-pwCVTZ		
C1	0.0000000000000000	0.0000000000000000	-0.03340773365122
H	0.0000000000000000	0.0000000000000000	1.23885047565122
2			
hf	FC-CCSD(T)/cc-pwCVDZ		
F	0.0000000000000000	0.0000000000000000	-0.04746242250823
H	0.0000000000000000	0.0000000000000000	0.87232813900823
2			
hf	FC-CCSD(T)/cc-pwCVQZ		
F	0.0000000000000000	0.0000000000000000	-0.04574671716658
H	0.0000000000000000	0.0000000000000000	0.87061243366658
2			
hf	FC-CCSD(T)/cc-pwCVTZ		
F	0.0000000000000000	0.0000000000000000	-0.04610566435226
H	0.0000000000000000	0.0000000000000000	0.87097138085226
2			
hf	CV-CCSD(T)/cc-pwCVDZ		
F	0.0000000000000000	0.0000000000000000	-0.04729214817865
H	0.0000000000000000	0.0000000000000000	0.87215786467865
2			
hf	CV-CCSD(T)/cc-pwCVQZ		
F	0.0000000000000000	0.0000000000000000	-0.04546061657295
H	0.0000000000000000	0.0000000000000000	0.87032633307295
2			
hf	CV-CCSD(T)/cc-pwCVTZ		
F	0.0000000000000000	0.0000000000000000	-0.04585622807206
H	0.0000000000000000	0.0000000000000000	0.87072194457206
2			
hs	FC-CCSD(T)/cc-pwCVDZ		

S	0.0000000000000000	0.0000000000000000	-0.04667602170638
H	0.0000000000000000	0.0000000000000000	1.30688984090638
2			
hs FC-CCSD(T)/cc-pwCVQZ			
S	0.0000000000000000	0.0000000000000000	-0.04064722786311
H	0.0000000000000000	0.0000000000000000	1.30086104706311
2			
hs FC-CCSD(T)/cc-pwCVTZ			
S	0.0000000000000000	0.0000000000000000	-0.04045847296413
H	0.0000000000000000	0.0000000000000000	1.30067229216413
2			
hs CV-CCSD(T)/cc-pwCVDZ			
S	0.0000000000000000	0.0000000000000000	-0.04659249217379
H	0.0000000000000000	0.0000000000000000	1.30680631137379
2			
hs CV-CCSD(T)/cc-pwCVQZ			
S	0.0000000000000000	0.0000000000000000	-0.03953963900988
H	0.0000000000000000	0.0000000000000000	1.29975345820988
2			
hs CV-CCSD(T)/cc-pwCVTZ			
S	0.0000000000000000	0.0000000000000000	-0.03956889140986
H	0.0000000000000000	0.0000000000000000	1.29978271060986
2			
n2 FC-CCSD(T)/cc-pwCVDZ			
N	0.0000000000000000	0.0000000000000000	-0.55858918971404
N	0.0000000000000000	0.0000000000000000	0.55858918971404
2			
n2 FC-CCSD(T)/cc-pwCVQZ			
N	0.0000000000000000	0.0000000000000000	-0.54997991369247
N	0.0000000000000000	0.0000000000000000	0.54997991369247
2			
n2 FC-CCSD(T)/cc-pwCVTZ			
N	0.0000000000000000	0.0000000000000000	-0.55081991204861
N	0.0000000000000000	0.0000000000000000	0.55081991204861
2			
n2 CV-CCSD(T)/cc-pwCVDZ			
N	0.0000000000000000	0.0000000000000000	-0.55829127994120
N	0.0000000000000000	0.0000000000000000	0.55829127994120
2			
n2 CV-CCSD(T)/cc-pwCVQZ			
N	0.0000000000000000	0.0000000000000000	-0.54896751138602
N	0.0000000000000000	0.0000000000000000	0.54896751138602
2			
n2 CV-CCSD(T)/cc-pwCVTZ			

N	0.0000000000000000	0.0000000000000000	-0.54996866227027
N	0.0000000000000000	0.0000000000000000	0.54996866227027
2			
nh	FC-CCSD(T)/cc-pwCVDZ		
N	0.0000000000000000	0.0000000000000000	-0.07888306883451
H	0.0000000000000000	0.0000000000000000	0.97659342553451
2			
nh	FC-CCSD(T)/cc-pwCVQZ		
N	0.0000000000000000	0.0000000000000000	-0.06976723853912
H	0.0000000000000000	0.0000000000000000	0.96747759523912
2			
nh	FC-CCSD(T)/cc-pwCVTZ		
N	0.0000000000000000	0.0000000000000000	-0.07043320162601
H	0.0000000000000000	0.0000000000000000	0.96814355832601
2			
nh	CV-CCSD(T)/cc-pwCVDZ		
N	0.0000000000000000	0.0000000000000000	-0.07855956379828
H	0.0000000000000000	0.0000000000000000	0.97626992049828
2			
nh	CV-CCSD(T)/cc-pwCVQZ		
N	0.0000000000000000	0.0000000000000000	-0.06915615394417
H	0.0000000000000000	0.0000000000000000	0.96686651064417
2			
nh	CV-CCSD(T)/cc-pwCVTZ		
N	0.0000000000000000	0.0000000000000000	-0.06989814541842
H	0.0000000000000000	0.0000000000000000	0.96760850211842
3			
nh2	FC-CCSD(T)/cc-pwCVDZ		
N	0.0000000000000000	0.00000000001339	-0.09761721736406
H	0.0000000000000000	0.80148725919925	0.56619843622671
H	0.0000000000000000	-0.80148725921264	0.56619843623735
3			
nh2	FC-CCSD(T)/cc-pwCVQZ		
N	0.0000000000000000	0.00000000001086	-0.08178901801669
H	0.0000000000000000	0.80065123487942	0.55828433655395
H	0.0000000000000000	-0.80065123489029	0.55828433656274
3			
nh2	FC-CCSD(T)/cc-pwCVTZ		
N	0.0000000000000000	0.00000000001655	-0.08437269456464
H	0.0000000000000000	0.79904144352007	0.55957617482552
H	0.0000000000000000	-0.79904144353662	0.55957617483912
3			
nh2	CV-CCSD(T)/cc-pwCVDZ		
N	0.0000000000000000	-0.00000000000447	-0.09700704341843

H	0.0000000000000000	0.80134915599527	0.56589334926128
H	0.0000000000000000	-0.80134915599080	0.56589334925714
3			
nh2	CV-CCSD(T)/cc-pwCVQZ		
N	0.0000000000000000	-0.000000000000485	-0.08063224120609
H	0.0000000000000000	0.80039596610447	0.55770594815500
H	0.0000000000000000	-0.80039596609962	0.55770594815109
3			
nh2	CV-CCSD(T)/cc-pwCVTZ		
N	0.0000000000000000	-0.000000000003756	-0.08333602926591
H	0.0000000000000000	0.79883913495484	0.55905784219813
H	0.0000000000000000	-0.79883913491727	0.55905784216778
4			
nh3	FC-CCSD(T)/cc-pwCVDZ		
N	0.00000339247595	0.000000000000297	0.10537430527957
H	0.93142427640429	0.000000000000543	-0.32715247093347
H	-0.46571383449568	-0.80663125407353	-0.32714646257421
H	-0.46571383448457	0.80663125406512	-0.32714646257189
4			
nh3	FC-CCSD(T)/cc-pwCVQZ		
N	-0.00000283496742	0.000000000001333	0.07247438868897
H	0.93486288953659	-0.000000000004769	-0.31618263536399
H	-0.46743002729713	-0.80961709477332	-0.31618142206574
H	-0.46743002737204	0.80961709480768	-0.31618142205924
4			
nh3	FC-CCSD(T)/cc-pwCVTZ		
N	-0.00000157082233	-0.000000000000645	0.07840858041443
H	0.93263546803305	0.000000000000256	-0.31816047825137
H	-0.46631694865572	-0.80768596138571	-0.31815959647991
H	-0.46631694865500	0.80768596138960	-0.31815959648315
4			
nh3	CV-CCSD(T)/cc-pwCVDZ		
N	0.00000124717936	-0.000000000000871	0.10415293996998
H	0.93136698268241	0.000000000001010	-0.32674464935370
H	-0.46568411498711	-0.80658469712220	-0.32673969070550
H	-0.46568411497466	0.80658469712082	-0.32673969071078
4			
nh3	CV-CCSD(T)/cc-pwCVQZ		
N	-0.00000387695093	0.000000000006804	0.07005950346680
H	0.93475087276996	-0.000000000007477	-0.31537793108658
H	-0.46737349791440	-0.80952200001989	-0.31537633160626
H	-0.46737349800463	0.80952200002662	-0.31537633157396
4			
nh3	CV-CCSD(T)/cc-pwCVTZ		

N	-0.00000289692663	0.00000000000138	0.07624372899336
H	0.93256484106298	0.00000000000889	-0.31743919704794
H	-0.46628097212628	-0.80762721302548	-0.31743781137299
H	-0.46628097211008	0.80762721301521	-0.31743781137243
2			
no FC-CCSD(T)/cc-pwCVDZ			
N	0.00000000000000	0.00000000000000	-0.61819233421728
O	0.00000000000000	0.00000000000000	0.54170668141728
2			
no FC-CCSD(T)/cc-pwCVQZ			
N	0.00000000000000	0.00000000000000	-0.61304242692893
O	0.00000000000000	0.00000000000000	0.53655677412893
2			
no FC-CCSD(T)/cc-pwCVTZ			
N	0.00000000000000	0.00000000000000	-0.61407711704471
O	0.00000000000000	0.00000000000000	0.53759146424471
2			
no CV-CCSD(T)/cc-pwCVDZ			
N	0.00000000000000	0.00000000000000	-0.61788218065430
O	0.00000000000000	0.00000000000000	0.54139652785430
2			
no CV-CCSD(T)/cc-pwCVQZ			
N	0.00000000000000	0.00000000000000	-0.61222282407040
O	0.00000000000000	0.00000000000000	0.53573717127040
2			
no CV-CCSD(T)/cc-pwCVTZ			
N	0.00000000000000	0.00000000000000	-0.61338067460266
O	0.00000000000000	0.00000000000000	0.53689502180266
2			
o2 FC-CCSD(T)/cc-pwCVDZ			
O	0.00000000000000	0.00000000000000	-0.60787036620059
O	0.00000000000000	0.00000000000000	0.60787036620059
2			
o2 FC-CCSD(T)/cc-pwCVQZ			
O	0.00000000000000	0.00000000000000	-0.60378981643206
O	0.00000000000000	0.00000000000000	0.60378981643206
2			
o2 FC-CCSD(T)/cc-pwCVTZ			
O	0.00000000000000	0.00000000000000	-0.60571721705857
O	0.00000000000000	0.00000000000000	0.60571721705857
2			
o2 CV-CCSD(T)/cc-pwCVDZ			
O	0.00000000000000	0.00000000000000	-0.60742162261922
O	0.00000000000000	0.00000000000000	0.60742162261922

2			
o2	CV-CCSD(T)/cc-pwCVQZ		
O	0.0000000000000000	0.0000000000000000	-0.60283397958405
O	0.0000000000000000	0.0000000000000000	0.60283397958405
2			
o2	CV-CCSD(T)/cc-pwCVTZ		
O	0.0000000000000000	0.0000000000000000	-0.60486608300195
O	0.0000000000000000	0.0000000000000000	0.60486608300195
2			
oh	FC-CCSD(T)/cc-pwCVDZ		
O	0.0000000000000000	0.0000000000000000	-0.06210806337357
H	0.0000000000000000	0.0000000000000000	0.91725733217357
2			
oh	FC-CCSD(T)/cc-pwCVQZ		
O	0.0000000000000000	0.0000000000000000	-0.05728351695143
H	0.0000000000000000	0.0000000000000000	0.91243278575143
2			
oh	FC-CCSD(T)/cc-pwCVTZ		
O	0.0000000000000000	0.0000000000000000	-0.05775721247440
H	0.0000000000000000	0.0000000000000000	0.91290648127440
2			
oh	CV-CCSD(T)/cc-pwCVDZ		
O	0.0000000000000000	0.0000000000000000	-0.06186533750347
H	0.0000000000000000	0.0000000000000000	0.91701460630347
2			
oh	CV-CCSD(T)/cc-pwCVQZ		
O	0.0000000000000000	0.0000000000000000	-0.05687103561785
H	0.0000000000000000	0.0000000000000000	0.91202030441785
2			
oh	CV-CCSD(T)/cc-pwCVTZ		
O	0.0000000000000000	0.0000000000000000	-0.05739688058924
H	0.0000000000000000	0.0000000000000000	0.91254614938924
2			
sih	FC-CCSD(T)/cc-pwCVDZ		
H	0.0000000000000000	0.0000000000000000	-1.47517378597734
Si	0.0000000000000000	0.0000000000000000	0.05874439497734
2			
sih	FC-CCSD(T)/cc-pwCVQZ		
H	0.0000000000000000	0.0000000000000000	-1.46896652337177
Si	0.0000000000000000	0.0000000000000000	0.05253713237177
2			
sih	FC-CCSD(T)/cc-pwCVTZ		
H	0.0000000000000000	0.0000000000000000	-1.46948179804212
Si	0.0000000000000000	0.0000000000000000	0.05305240704212

```
2
sih CV-CCSD(T)/cc-pwCVDZ
  H  0.000000000000000  0.000000000000000  -1.4759881962610
  Si 0.000000000000000  0.000000000000000   0.05916942862610
2
sih CV-CCSD(T)/cc-pwCVQZ
  H  0.000000000000000  0.000000000000000  -1.46723561349233
  Si 0.000000000000000  0.000000000000000   0.05080622249233
2
sih CV-CCSD(T)/cc-pwCVTZ
  H  0.000000000000000  0.000000000000000  -1.46807846514786
  Si 0.000000000000000  0.000000000000000   0.05164907414786
```

Raw Energies

Table S16. Raw data for SD(T)/nZ (n = D, T, Q, 5) computations. System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons ($N_{\text{val_el}}$), number of basis functions (Basis size), time for SD(T) computation, (Time SD(T)), time for SD computation (Time SD), and energy components in Hartree (HF, CCSD, CCSD(T)) are provided.

System	CV	Cardinal	M	N_{el}	$N_{\text{val_el}}$	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
alcl	CV	2	1	30	10	54	0.024	0.02	-701.48743452	-701.97769775	-701.98602345
alcl	CV	3	1	30	10	118	0.277	0.22	-701.51217072	-702.36124841	-702.37855580
alcl	CV	4	1	30	10	218	2.215	1.339	-701.51722646	-702.53252070	-702.55330936
alcl	CV	5	1	30	10	362	12.504	6.814	-701.51804827	-702.60820571	-702.63014479
alcl	FC	2	1	30	10	54	0.004	0.004	-701.48743452	-701.69756399	-701.70286173
alcl	FC	3	1	30	10	118	0.058	0.054	-701.51217072	-701.78362249	-701.79517553
alcl	FC	4	1	30	10	218	0.593	0.556	-701.51722646	-701.80891571	-701.82241347
alcl	FC	5	1	30	10	362	4.144	3.915	-701.51804827	-701.81578132	-701.82987655
alf	CV	2	1	22	10	45	0.012	0.01	-341.42636493	-341.84377089	-341.85051592
alf	CV	3	1	22	10	102	0.112	0.097	-341.47411961	-342.13260963	-342.14601608
alf	CV	4	1	22	10	193	0.932	0.71	-341.48547488	-342.24207562	-342.25792134
alf	CV	5	1	22	10	326	5.912	4.374	-341.48788483	-342.28853697	-342.30523665
alf	FC	2	1	22	10	45	0.003	0.003	-341.42636493	-341.68304390	-341.68785179
alf	FC	3	1	22	10	102	0.04	0.038	-341.47411961	-341.80052560	-341.81033343
alf	FC	4	1	22	10	193	0.414	0.391	-341.48547488	-341.83363505	-341.84490728
alf	FC	5	1	22	10	326	3.235	3.079	-341.48788483	-341.84381151	-341.85557730
alh	CV	2	1	14	4	32	0.003	0.003	-242.45506546	-242.65895537	-242.66184318
alh	CV	3	1	14	4	73	0.021	0.019	-242.46258102	-242.82196422	-242.82674922
alh	CV	4	1	14	4	139	0.149	0.134	-242.46423867	-242.89536749	-242.90120674
alh	CV	5	1	14	4	236	0.966	0.828	-242.46457579	-242.93047397	-242.93668901
alh	FC	2	1	14	4	32	0.001	0.001	-242.45506546	-242.52920217	-242.53022690
alh	FC	3	1	14	4	73	0.007	0.007	-242.46258102	-242.54532239	-242.54676769
alh	FC	4	1	14	4	139	0.078	0.077	-242.46423867	-242.54919683	-242.55078975
alh	FC	5	1	14	4	236	0.612	0.607	-242.46457579	-242.55005943	-242.55168839
alh3	CV	2	1	16	6	42	0.006	0.005	-243.63483211	-243.86441299	-243.86711139
alh3	CV	3	1	16	6	101	0.062	0.054	-243.64655604	-244.04054779	-244.04487549
alh3	CV	4	1	16	6	199	0.556	0.439	-243.64926999	-244.11717104	-244.12252480
alh3	CV	5	1	16	6	346	3.624	2.831	-243.64972315	-244.15291859	-244.15864310

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
alh3	FC	2	1	16	6	42	0.002	0.002	-243.63483211	-243.73625204	-243.73738078
alh3	FC	3	1	16	6	101	0.025	0.025	-243.64655604	-243.76437007	-243.76595385
alh3	FC	4	1	16	6	199	0.329	0.322	-243.64926999	-243.77131553	-243.77306660
alh3	FC	5	1	16	6	346	2.689	2.639	-243.64972315	-243.77278216	-243.77457728
bf	CV	2	1	14	10	36	0.004	0.004	-124.10797240	-124.44236471	-124.44934302
bf	CV	3	1	14	10	86	0.035	0.031	-124.15691173	-124.59849891	-124.61080035
bf	CV	4	1	14	10	168	0.314	0.276	-124.16598520	-124.64017722	-124.65376861
bf	CV	5	1	14	10	290	2.089	1.801	-124.16832541	-124.65338789	-124.66742300
bf	FC	2	1	14	10	36	0.002	0.002	-124.10797240	-124.38342834	-124.39005023
bf	FC	3	1	14	10	86	0.024	0.023	-124.15691173	-124.49958663	-124.51109742
bf	FC	4	1	14	10	168	0.282	0.267	-124.16598520	-124.52948713	-124.54217465
bf	FC	5	1	14	10	290	2.097	1.986	-124.16832541	-124.53927173	-124.55237472
bh	CV	2	1	6	4	23	0.001	0.001	-25.12552999	-25.24254686	-25.24424148
bh	CV	3	1	6	4	57	0.005	0.004	-25.13010666	-25.27312305	-25.27575010
bh	CV	4	1	6	4	114	0.05	0.049	-25.13133371	-25.28165309	-25.28447264
bh	CV	5	1	6	4	200	0.428	0.42	-25.13156523	-25.28400207	-25.28687896
bh	FC	2	1	6	4	23	0.001	0.001	-25.12552999	-25.21491106	-25.21632444
bh	FC	3	1	6	4	57	0.004	0.004	-25.13010666	-25.22969058	-25.23179473
bh	FC	4	1	6	4	114	0.042	0.041	-25.13133371	-25.23316006	-25.23540306
bh	FC	5	1	6	4	200	0.541	0.538	-25.13156523	-25.23405244	-25.23633944
bh3	CV	2	1	8	6	33	0.002	0.002	-26.39131984	-26.53702172	-26.53876304
bh3	CV	3	1	8	6	85	0.017	0.017	-26.40044066	-26.58147356	-26.58437733
bh3	CV	4	1	8	6	174	0.23	0.22	-26.40216418	-26.59278324	-26.59593659
bh3	CV	5	1	8	6	310	1.966	1.887	-26.40255734	-26.59590766	-26.59913375
bh3	FC	2	1	8	6	33	0.001	0.001	-26.39131984	-26.50863137	-26.51023014
bh3	FC	3	1	8	6	85	0.015	0.014	-26.40044066	-26.53652671	-26.53913096
bh3	FC	4	1	8	6	174	0.211	0.205	-26.40216418	-26.54263591	-26.54544450
bh3	FC	5	1	8	6	310	1.838	1.802	-26.40255734	-26.54426778	-26.54713798
c2h2	CV	2	1	14	10	46	0.006	0.005	-76.82720436	-77.16466299	-77.17685295
c2h2	CV	3	1	14	10	114	0.084	0.076	-76.84989800	-77.27171409	-77.28953026
c2h2	CV	4	1	14	10	228	0.856	0.731	-76.85426105	-77.30007012	-77.31905369
c2h2	CV	5	1	14	10	400	6.371	5.303	-76.85525538	-77.30847742	-77.32783020
c2h2	FC	2	1	14	10	46	0.004	0.004	-76.82720436	-77.10443718	-77.11619100
c2h2	FC	3	1	14	10	114	0.061	0.057	-76.84989800	-77.17560411	-77.19249788

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
c2h2	FC	4	1	14	10	228	0.795	0.747	-76.85426105	-77.19295490	-77.21089098
c2h2	FC	5	1	14	10	400	6.689	6.289	-76.85525538	-77.19818662	-77.21646252
c2h3f	CV	2	1	24	18	69	0.037	0.032	-176.89661610	-177.47946549	-177.49426889
c2h3f	CV	3	1	24	18	171	0.691	0.515	-176.95431818	-177.70985308	-177.73455332
c2h3f	CV	4	1	24	18	342	7.504	5.095	-176.96741978	-177.77326954	-177.80032402
c2h3f	CV	5	1	24	18	600	78.646	56.099	-176.97084744	-177.79312419	-177.82098034
c2h3f	FC	2	1	24	18	69	0.023	0.021	-176.89661610	-177.38806230	-177.40230797
c2h3f	FC	3	1	24	18	171	0.453	0.375	-176.95431818	-177.55892428	-177.58239653
c2h3f	FC	4	1	24	18	342	4.964	3.925	-176.96741978	-177.60480464	-177.63044754
c2h3f	FC	5	1	24	18	600	54.555	45	-176.97084744	-177.61956450	-177.64596456
c2h4	CV	2	1	16	12	56	0.01	0.009	-78.04097902	-78.41070840	-78.42146853
c2h4	CV	3	1	16	12	142	0.166	0.14	-78.06435059	-78.52394214	-78.54018133
c2h4	CV	4	1	16	12	288	2.114	1.707	-78.06924606	-78.55386348	-78.57128837
c2h4	CV	5	1	16	12	510	22.109	18.012	-78.07043905	-78.56262932	-78.58042015
c2h4	FC	2	1	16	12	56	0.007	0.007	-78.04097902	-78.35030269	-78.36065267
c2h4	FC	3	1	16	12	142	0.139	0.128	-78.06435059	-78.42784603	-78.44323470
c2h4	FC	4	1	16	12	288	1.744	1.567	-78.06924606	-78.44681352	-78.46327102
c2h4	FC	5	1	16	12	510	20.156	18.411	-78.07043905	-78.45241844	-78.46921485
cch	CV	2	2	13	9	41	0.017	0.015	-76.15856253	-76.45454280	-76.46550457
cch	CV	3	2	13	9	100	0.61	0.577	-76.17833456	-76.55266386	-76.56885822
cch	CV	4	2	13	9	198	9.709	9.309	-76.18244731	-76.57916459	-76.59647285
cch	CV	5	2	13	9	345	112.289	109.052	-76.18334206	-76.58704815	-76.60471790
cch	FC	2	2	13	9	41	0.015	0.014	-76.15856253	-76.39478142	-76.40528403
cch	FC	3	2	13	9	100	0.513	0.497	-76.17833456	-76.45711823	-76.47236167
cch	FC	4	2	13	9	198	9.029	8.845	-76.18244731	-76.47265224	-76.48888438
cch	FC	5	2	13	9	345	105.893	104.604	-76.18334206	-76.47737285	-76.49393696
cc12	CV	2	1	40	18	72	0.087	0.071	-956.76896301	-957.53462782	-957.55390078
cc12	CV	3	1	40	18	161	1.354	0.862	-956.80970936	-958.01926242	-958.05500135
cc12	CV	4	1	40	18	302	12.112	5.831	-956.81937586	-958.22635832	-958.26725669
cc12	CV	5	1	40	18	507	101.036	44.793	-956.82096833	-958.31098463	-958.35357312
cc12	FC	2	1	40	18	72	0.018	0.016	-956.76896301	-957.20560183	-957.22201535
cc12	FC	3	1	40	18	161	0.31	0.262	-956.80970936	-957.37163156	-957.40165488
cc12	FC	4	1	40	18	302	2.864	2.267	-956.81937586	-957.42069545	-957.45453062
cc12	FC	5	1	40	18	507	28.058	22.813	-956.82096833	-957.43467598	-957.46974976

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
cf	CV	2	2	15	11	36	0.012	0.01	-137.18045979	-137.53899640	-137.54710121
cf	CV	3	2	15	11	86	0.284	0.26	-137.22542867	-137.70191830	-137.71626947
cf	CV	4	2	15	11	168	4.15	3.869	-137.23574179	-137.74694180	-137.76281365
cf	CV	5	2	15	11	290	47.101	44.372	-137.23848787	-137.76139280	-137.77779732
cf	FC	2	2	15	11	36	0.008	0.007	-137.18045979	-137.47873664	-137.48651075
cf	FC	3	2	15	11	86	0.254	0.24	-137.22542867	-137.60035045	-137.61394336
cf	FC	4	2	15	11	168	3.947	3.805	-137.23574179	-137.63340248	-137.64840163
cf	FC	5	2	15	11	290	45.921	44.715	-137.23848787	-137.64436619	-137.65987044
cf2	CV	2	1	24	18	54	0.02	0.017	-236.67370303	-237.28146974	-237.29534730
cf2	CV	3	1	24	18	129	0.261	0.212	-236.75566954	-237.56850999	-237.59346016
cf2	CV	4	1	24	18	252	2.683	1.894	-236.77427481	-237.64841724	-237.67616499
cf2	CV	5	1	24	18	435	19.437	12.425	-236.77924305	-237.67436739	-237.70312009
cf2	FC	2	1	24	18	54	0.011	0.01	-236.67370303	-237.19005650	-237.20343518
cf2	FC	3	1	24	18	129	0.163	0.142	-236.75566954	-237.41201904	-237.43580021
cf2	FC	4	1	24	18	252	1.711	1.374	-236.77427481	-237.47337583	-237.49977103
cf2	FC	5	1	24	18	435	12.585	9.631	-236.77924305	-237.49390554	-237.52126040
ch	CV	2	2	7	5	23	0.003	0.003	-38.27278717	-38.40974415	-38.41187495
ch	CV	3	2	7	5	57	0.049	0.046	-38.28152217	-38.45547299	-38.45929131
ch	CV	4	2	7	5	114	0.809	0.789	-38.28378371	-38.46764908	-38.47185971
ch	CV	5	2	7	5	200	8.227	8.108	-38.28433904	-38.47118475	-38.47551683
ch	FC	2	2	7	5	23	0.003	0.003	-38.27278717	-38.38054181	-38.38246574
ch	FC	3	2	7	5	57	0.046	0.045	-38.28152217	-38.40892012	-38.41232820
ch	FC	4	2	7	5	114	0.852	0.84	-38.28378371	-38.41573577	-38.41948509
ch	FC	5	2	7	5	200	8.229	8.159	-38.28433904	-38.41772458	-38.42158369
ch2c	CV	2	1	14	10	46	0.007	0.006	-76.77432688	-77.10003920	-77.11044677
ch2c	CV	3	1	14	10	114	0.101	0.093	-76.79433596	-77.20232713	-77.21782426
ch2c	CV	4	1	14	10	228	0.973	0.842	-76.79880507	-77.22991901	-77.24652766
ch2c	CV	5	1	14	10	400	7.157	6.061	-76.79984691	-77.23808964	-77.25505897
ch2c	FC	2	1	14	10	46	0.004	0.004	-76.77432688	-77.04036213	-77.05033253
ch2c	FC	3	1	14	10	114	0.076	0.073	-76.79433596	-77.10715099	-77.12175352
ch2c	FC	4	1	14	10	228	0.915	0.865	-76.79880507	-77.12383550	-77.13943088
ch2c	FC	5	1	14	10	400	7.581	7.17	-76.79984691	-77.12885900	-77.14478723
ch2ch	CV	2	2	15	11	51	0.04	0.035	-77.39919570	-77.73121864	-77.74096624
ch2ch	CV	3	2	15	11	128	1.517	1.425	-77.42073732	-77.83841391	-77.85331593

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
ch2ch	CV	4	2	15	11	258	28.112	26.402	-77.42538301	-77.86701751	-77.88307701
ch2ch	CV	5	2	15	11	455	424.079	411.496	-77.42646791	-77.87541145	-77.89183712
ch2ch	FC	2	2	15	11	51	0.032	0.029	-77.39919570	-77.67108795	-77.68043242
ch2ch	FC	3	2	15	11	128	1.433	1.381	-77.42073732	-77.74259750	-77.75666524
ch2ch	FC	4	2	15	11	258	27.328	26.558	-77.42538301	-77.76025849	-77.77536869
ch2ch	FC	5	2	15	11	455	420.273	414.859	-77.42646791	-77.76549585	-77.78094543
ch2nh	CV	2	1	16	12	51	0.01	0.009	-94.03973426	-94.43134879	-94.44298800
ch2nh	CV	3	1	16	12	128	0.143	0.129	-94.06781976	-94.55926329	-94.57734797
ch2nh	CV	4	1	16	12	258	1.482	1.186	-94.07451276	-94.59423003	-94.61374272
ch2nh	CV	5	1	16	12	455	11.939	9.312	-94.07615183	-94.60471328	-94.62469489
ch2nh	FC	2	1	16	12	51	0.006	0.006	-94.03973426	-94.37065913	-94.38188463
ch2nh	FC	3	1	16	12	128	0.102	0.095	-94.06781976	-94.46113382	-94.47833387
ch2nh	FC	4	1	16	12	258	1.25	1.121	-94.07451276	-94.48485029	-94.50335511
ch2nh	FC	5	1	16	12	455	10.574	9.461	-94.07615183	-94.49210427	-94.51104884
ch2nh2	CV	2	2	17	13	56	0.056	0.048	-94.60051824	-94.99229787	-95.00112317
ch2nh2	CV	3	2	17	13	142	2.239	2.054	-94.63112809	-95.12767397	-95.14293421
ch2nh2	CV	4	2	17	13	288	47.623	44.139	-94.63834294	-95.16433130	-95.18107696
ch2nh2	CV	5	2	17	13	510	711.333	685.542	-94.64036766	-95.17552503	-95.19277226
ch2nh2	FC	2	2	17	13	56	0.046	0.042	-94.60051824	-94.93127135	-94.93974741
ch2nh2	FC	3	2	17	13	142	2.129	2.025	-94.63112809	-95.02912745	-95.04362357
ch2nh2	FC	4	2	17	13	288	45.043	43.376	-94.63834294	-95.05452816	-95.07039502
ch2nh2	FC	5	2	17	13	510	662.936	650.732	-94.64036766	-95.06249631	-95.07883723
ch2-sing	CV	2	1	8	6	28	0.002	0.001	-38.88143268	-39.05133856	-39.05462717
ch2-sing	CV	3	1	8	6	71	0.012	0.012	-38.89256998	-39.10532384	-39.11073659
ch2-sing	CV	4	1	8	6	144	0.136	0.13	-38.89517009	-39.11948718	-39.12540203
ch2-sing	CV	5	1	8	6	255	1.114	1.071	-38.89585672	-39.12362071	-39.12969229
ch2-sing	FC	2	1	8	6	28	0.001	0.001	-38.88143268	-39.02187633	-39.02492636
ch2-sing	FC	3	1	8	6	71	0.01	0.01	-38.89256998	-39.05842200	-39.06338185
ch2-sing	FC	4	1	8	6	144	0.12	0.118	-38.89517009	-39.06719566	-39.07260377
ch2-sing	FC	5	1	8	6	255	1.05	1.031	-38.89585672	-39.06977374	-39.07532648
ch2-trip	CV	2	3	8	6	28	0.004	0.004	-38.92711624	-39.07182794	-39.07382440
ch2-trip	CV	3	3	8	6	71	0.122	0.116	-38.93792252	-39.12377946	-39.12758515
ch2-trip	CV	4	3	8	6	144	2.151	2.101	-38.94026082	-39.13710189	-39.14133833
ch2-trip	CV	5	3	8	6	255	21.054	20.696	-38.94083973	-39.14093134	-39.14529619

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
ch2-trip	FC	2	3	8	6	28	0.004	0.003	-38.92711624	-39.04203369	-39.04389787
ch2-trip	FC	3	3	8	6	71	0.109	0.105	-38.93792252	-39.07618379	-39.07970019
ch2-trip	FC	4	3	8	6	144	2.024	1.992	-38.94026082	-39.08405484	-39.08795587
ch2-trip	FC	5	3	8	6	255	19.974	19.768	-38.94083973	-39.08631392	-39.09033266
ch3	CV	2	2	9	7	33	0.006	0.005	-39.56429682	-39.74582902	-39.74875663
ch3	CV	3	2	9	7	85	0.224	0.213	-39.57776830	-39.80603994	-39.81123460
ch3	CV	4	2	9	7	174	4.106	3.987	-39.58037970	-39.82120716	-39.82692422
ch3	CV	5	2	9	7	310	50.013	49.06	-39.58105650	-39.82559877	-39.83147174
ch3	FC	2	2	9	7	33	0.005	0.005	-39.56429682	-39.71570634	-39.71847719
ch3	FC	3	2	9	7	85	0.213	0.205	-39.57776830	-39.75808935	-39.76295124
ch3	FC	4	2	9	7	174	4.067	3.99	-39.58037970	-39.76778641	-39.77311978
ch3	FC	5	2	9	7	310	49.833	49.285	-39.58105650	-39.77060204	-39.77607944
ch3f	CV	2	1	18	14	51	0.011	0.01	-139.04550410	-139.47226894	-139.47974532
ch3f	CV	3	1	18	14	128	0.162	0.139	-139.09489582	-139.65601095	-139.67052735
ch3f	CV	4	1	18	14	258	1.788	1.354	-139.10624491	-139.70663179	-139.72297612
ch3f	CV	5	1	18	14	455	13.83	10.156	-139.10935102	-139.72267996	-139.73965699
ch3f	FC	2	1	18	14	51	0.007	0.007	-139.04550410	-139.41101284	-139.41816987
ch3f	FC	3	1	18	14	128	0.12	0.108	-139.09489582	-139.55316487	-139.56694731
ch3f	FC	4	1	18	14	258	1.297	1.089	-139.10624491	-139.59174131	-139.60723211
ch3f	FC	5	1	18	14	455	9.985	8.23	-139.10935102	-139.60428008	-139.62037382
ch3nh	CV	2	2	17	13	56	0.053	0.045	-94.60262299	-94.98662273	-94.99492759
ch3nh	CV	3	2	17	13	142	2.224	2.044	-94.63139068	-95.11840549	-95.13264558
ch3nh	CV	4	2	17	13	288	45.182	41.697	-94.63810084	-95.15393630	-95.16957136
ch3nh	CV	5	2	17	13	510	698.696	663.058	-94.63982274	-95.16458493	-95.18068094
ch3nh	FC	2	2	17	13	56	0.043	0.038	-94.60262299	-94.92585687	-94.93381416
ch3nh	FC	3	2	17	13	142	2.132	2.028	-94.63139068	-95.02027498	-95.03375669
ch3nh	FC	4	2	17	13	288	42.98	41.312	-94.63810084	-95.04458217	-95.05934493
ch3nh	FC	5	2	17	13	510	686.631	670.905	-94.63982274	-95.05201033	-95.06720671
ch3nh2	CV	2	1	18	14	61	0.016	0.014	-95.22258932	-95.64519129	-95.65456068
ch3nh2	CV	3	1	18	14	156	0.323	0.267	-95.25379676	-95.78522455	-95.80121918
ch3nh2	CV	4	1	18	14	318	3.879	2.998	-95.26091262	-95.82285501	-95.84036172
ch3nh2	CV	5	1	18	14	565	42.844	34.541	-95.26283664	-95.83420454	-95.85220541
ch3nh2	FC	2	1	18	14	61	0.011	0.01	-95.22258932	-95.58407553	-95.59308528
ch3nh2	FC	3	1	18	14	156	0.241	0.213	-95.25379676	-95.68670051	-95.70191564

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
ch3nh2	FC	4	1	18	14	318	2.84	2.413	-95.26091262	-95.71308558	-95.72969642
ch3nh2	FC	5	1	18	14	565	33.945	29.987	-95.26283664	-95.72120803	-95.73828495
ch4	CV	2	1	10	8	38	0.002	0.002	-40.19927119	-40.41629695	-40.42038215
ch4	CV	3	1	10	8	99	0.035	0.032	-40.21367721	-40.48193028	-40.48872601
ch4	CV	4	1	10	8	204	0.475	0.438	-40.21628199	-40.49831278	-40.50570033
ch4	CV	5	1	10	8	365	4.043	3.78	-40.21696634	-40.50301282	-40.51056607
ch4	FC	2	1	10	8	38	0.002	0.002	-40.19927119	-40.38590669	-40.38982031
ch4	FC	3	1	10	8	99	0.028	0.027	-40.21367721	-40.43369912	-40.44013748
ch4	FC	4	1	10	8	204	0.386	0.364	-40.21628199	-40.44459447	-40.45157121
ch4	FC	5	1	10	8	365	3.422	3.282	-40.21696634	-40.44771207	-40.45484225
c-hcoh	CV	2	1	16	12	46	0.008	0.007	-113.79253313	-114.18782665	-114.19806287
c-hcoh	CV	3	1	16	12	114	0.11	0.099	-113.82794071	-114.33472183	-114.35190094
c-hcoh	CV	4	1	16	12	228	1.011	0.832	-113.83635745	-114.37527481	-114.39402761
c-hcoh	CV	5	1	16	12	400	8.081	6.604	-113.83844613	-114.38777090	-114.40705490
c-hcoh	FC	2	1	16	12	46	0.005	0.005	-113.79253313	-114.12747375	-114.13732731
c-hcoh	FC	3	1	16	12	114	0.077	0.072	-113.82794071	-114.23505330	-114.25138918
c-hcoh	FC	4	1	16	12	228	0.846	0.766	-113.83635745	-114.26403780	-114.28182669
c-hcoh	FC	5	1	16	12	400	7.095	6.46	-113.83844613	-114.27316951	-114.29146068
c-hono	CV	2	1	24	18	59	0.029	0.026	-204.66044196	-205.31725725	-205.33913320
c-hono	CV	3	1	24	18	143	0.422	0.34	-204.72351915	-205.56831470	-205.60317185
c-hono	CV	4	1	24	18	282	4.149	2.949	-204.73886108	-205.63924582	-205.67714338
c-hono	CV	5	1	24	18	490	51.56	40.445	-204.74253919	-205.66153666	-205.70051219
c-hono	FC	2	1	24	18	59	0.017	0.015	-204.66044196	-205.22580096	-205.24706589
c-hono	FC	3	1	24	18	143	0.275	0.239	-204.72351915	-205.41384855	-205.44731527
c-hono	FC	4	1	24	18	282	2.755	2.239	-204.73886108	-205.46675446	-205.50305744
c-hono	FC	5	1	24	18	490	38.289	33.529	-204.74253919	-205.48380792	-205.52113864
cl2	CV	2	1	34	14	54	0.027	0.022	-918.96547262	-919.57541556	-919.58561213
cl2	CV	3	1	34	14	118	0.31	0.233	-919.00165471	-920.02115669	-920.04501812
cl2	CV	4	1	34	14	218	2.595	1.378	-919.00917320	-920.21511260	-920.24363481
cl2	CV	5	1	34	14	362	15.382	7.351	-919.01038800	-920.29578998	-920.32577726
cl2	FC	2	1	34	14	54	0.005	0.005	-918.96547262	-919.27597290	-919.28357580
cl2	FC	3	1	34	14	118	0.073	0.067	-919.00165471	-919.42052699	-919.43915265
cl2	FC	4	1	34	14	218	0.624	0.534	-919.00917320	-919.46178169	-919.48377604
cl2	FC	5	1	34	14	362	3.922	3.333	-919.01038800	-919.47337412	-919.49639772

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
clcn	CV	2	1	30	16	63	0.037	0.032	-551.79327128	-552.44827312	-552.46819220
clcn	CV	3	1	30	16	145	0.549	0.402	-551.83322431	-552.78055207	-552.81356146
clcn	CV	4	1	30	16	277	4.916	2.895	-551.84191601	-552.90802300	-552.94454374
clcn	CV	5	1	30	16	471	84.904	69.21	-551.84356342	-552.95765536	-552.99532321
clcn	FC	2	1	30	16	63	0.012	0.011	-551.79327128	-552.23790317	-552.25610633
clcn	FC	3	1	30	16	145	0.177	0.154	-551.83322431	-552.38194117	-552.41144367
clcn	FC	4	1	30	16	277	1.811	1.491	-551.84191601	-552.42180141	-552.45404649
clcn	FC	5	1	30	16	471	43.766	41.293	-551.84356342	-552.43364985	-552.46679397
clf	CV	2	1	26	14	45	0.014	0.013	-558.84792732	-559.38601784	-559.39521433
clf	CV	3	1	26	14	102	0.14	0.117	-558.90328560	-559.73149157	-559.75194367
clf	CV	4	1	26	14	193	1.064	0.751	-558.91653886	-559.86311454	-559.88714425
clf	CV	5	1	26	14	326	7.186	4.708	-558.91962671	-559.91474993	-559.93997725
clf	FC	2	1	26	14	45	0.005	0.004	-558.84792732	-559.20543709	-559.21317344
clf	FC	3	1	26	14	102	0.052	0.047	-558.90328560	-559.37647941	-559.39393855
clf	FC	4	1	26	14	193	0.431	0.377	-558.91653886	-559.42517640	-559.44550027
clf	FC	5	1	26	14	326	2.942	2.542	-558.91962671	-559.44034578	-559.46163070
clo	CV	2	2	25	13	45	0.034	0.025	-534.26045464	-534.76349051	-534.77356814
clo	CV	3	2	25	13	102	0.714	0.604	-534.30642296	-535.08200030	-535.10309789
clo	CV	4	2	25	13	193	9.572	7.91	-534.31635341	-535.20430502	-535.22885119
clo	CV	5	2	25	13	326	93.705	77.606	-534.31861331	-535.25296117	-535.27866586
clo	FC	2	2	25	13	45	0.014	0.013	-534.26045464	-534.58334506	-534.59192298
clo	FC	3	2	25	13	102	0.491	0.463	-534.30642296	-534.72947065	-534.74747855
clo	FC	4	2	25	13	193	7.129	6.823	-534.31635341	-534.76929544	-534.79002256
clo	FC	5	2	25	13	326	74.554	72.042	-534.31861331	-534.78162882	-534.80327187
cn	CV	2	2	13	9	36	0.013	0.012	-92.21375638	-92.54343833	-92.55715274
cn	CV	3	2	13	9	86	0.313	0.293	-92.19260241	-92.60809382	-92.62739551
cn	CV	4	2	13	9	168	4.716	4.503	-92.19700024	-92.63497408	-92.65502713
cn	CV	5	2	13	9	290	49.635	47.873	-92.20816397	-92.65653202	-92.67693278
cn	FC	2	2	13	9	36	0.01	0.009	-92.21375638	-92.48365773	-92.49685952
cn	FC	3	2	13	9	86	0.277	0.266	-92.19260241	-92.51096727	-92.52927158
cn	FC	4	2	13	9	168	4.363	4.262	-92.19700024	-92.52653083	-92.54548389
cn	FC	5	2	13	9	290	46.941	46.222	-92.20816397	-92.54473905	-92.56401697
c-n2h2	CV	2	1	16	12	46	0.007	0.007	-109.99748235	-110.41608391	-110.42934315
c-n2h2	CV	3	1	16	12	114	0.104	0.093	-110.02927179	-110.55659398	-110.57742559

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
c-n2h2	CV	4	1	16	12	228	0.955	0.774	-110.03743494	-110.59588308	-110.61840615
c-n2h2	CV	5	1	16	12	400	7.772	6.294	-110.03942886	-110.60789702	-110.63100808
c-n2h2	FC	2	1	16	12	46	0.005	0.004	-109.99748235	-110.35524891	-110.36807176
c-n2h2	FC	3	1	16	12	114	0.072	0.067	-110.02927179	-110.45659825	-110.47648258
c-n2h2	FC	4	1	16	12	228	0.847	0.766	-110.03743494	-110.48436454	-110.50581019
c-n2h2	FC	5	1	16	12	400	6.695	6.062	-110.03942886	-110.49308714	-110.51508984
co	CV	2	1	14	10	36	0.004	0.003	-112.74982522	-113.11313762	-113.12507272
co	CV	3	1	14	10	86	0.035	0.032	-112.78123530	-113.24596225	-113.26442563
co	CV	4	1	14	10	168	0.3	0.262	-112.78873241	-113.28348814	-113.30334795
co	CV	5	1	14	10	290	1.99	1.703	-112.79035975	-113.29500239	-113.31533030
co	FC	2	1	14	10	36	0.002	0.002	-112.74982522	-113.05300830	-113.06455638
co	FC	3	1	14	10	86	0.024	0.022	-112.78123530	-113.14623147	-113.16381413
co	FC	4	1	14	10	168	0.262	0.247	-112.78873241	-113.17211164	-113.19096293
co	FC	5	1	14	10	290	1.961	1.851	-112.79035975	-113.18023823	-113.19952658
co2	CV	2	1	22	16	54	0.017	0.014	-187.65177136	-188.23560721	-188.25558799
co2	CV	3	1	22	16	129	0.221	0.183	-187.70829915	-188.46404202	-188.49484434
co2	CV	4	1	22	16	252	2.277	1.659	-187.72160976	-188.52885405	-188.56213438
co2	CV	5	1	22	16	435	16.866	11.775	-187.72458802	-188.54890379	-188.58302476
co2	FC	2	1	22	16	54	0.009	0.008	-187.65177136	-188.14420679	-188.16362186
co2	FC	3	1	22	16	129	0.135	0.119	-187.70829915	-188.31102719	-188.34052418
co2	FC	4	1	22	16	252	1.297	1.054	-187.72160976	-188.35797388	-188.38975109
co2	FC	5	1	22	16	435	9.728	7.778	-187.72458802	-188.37281368	-188.40538261
cs	CV	2	1	22	10	45	0.012	0.011	-435.33407383	-435.77998013	-435.79702124
cs	CV	3	1	22	10	102	0.114	0.099	-435.35552709	-436.01908956	-436.04447933
cs	CV	4	1	22	10	193	0.917	0.682	-435.36088764	-436.12225900	-436.15007087
cs	CV	5	1	22	10	326	5.756	4.14	-435.36181555	-436.16410638	-436.19272744
cs	FC	2	1	22	10	45	0.003	0.003	-435.33407383	-435.60140142	-435.61663988
cs	FC	3	1	22	10	102	0.04	0.038	-435.35552709	-435.67890009	-435.70085526
cs	FC	4	1	22	10	193	0.43	0.402	-435.36088764	-435.70042955	-435.72403154
cs	FC	5	1	22	10	326	3.144	2.98	-435.36181555	-435.70679138	-435.73094459
cs2	CV	2	1	38	16	72	0.077	0.062	-832.93497425	-833.67925709	-833.70672157
cs2	CV	3	1	38	16	161	1.187	0.736	-832.97270605	-834.12051961	-834.16264109
cs2	CV	4	1	38	16	302	10.99	5.315	-832.98095724	-834.31526474	-834.36188286
cs2	CV	5	1	38	16	507	78.478	35.491	-832.98225534	-834.39527251	-834.44333743

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
cs2	FC	2	1	38	16	72	0.014	0.012	-832.93497425	-833.35050732	-833.37476733
cs2	FC	3	1	38	16	161	0.22	0.186	-832.97270605	-833.48598560	-833.52200755
cs2	FC	4	1	38	16	302	2.281	1.845	-832.98095724	-833.52286781	-833.56193034
cs2	FC	5	1	38	16	507	21.267	17.936	-832.98225534	-833.53349576	-833.57351681
dioxirane	CV	2	1	24	18	64	0.031	0.027	-188.61775918	-189.25044884	-189.26982890
dioxirane	CV	3	1	24	18	157	0.552	0.423	-188.67825961	-189.49160093	-189.52316326
dioxirane	CV	4	1	24	18	312	5.766	3.981	-188.69160552	-189.55753713	-189.59199230
dioxirane	CV	5	1	24	18	545	58.17	40.441	-188.69503694	-189.57847726	-189.61394500
dioxirane	FC	2	1	24	18	64	0.019	0.017	-188.61775918	-189.15928479	-189.17802959
dioxirane	FC	3	1	24	18	157	0.363	0.303	-188.67825961	-189.33941016	-189.36956892
dioxirane	FC	4	1	24	18	312	3.767	3.001	-188.69160552	-189.38765733	-189.42050662
dioxirane	FC	5	1	24	18	545	40.861	33.24	-188.69503694	-189.40344265	-189.43725419
f2	CV	2	1	18	14	36	0.006	0.005	-198.68616632	-199.16592302	-199.17634038
f2	CV	3	1	18	14	86	0.046	0.04	-198.75273797	-199.40081275	-199.42053187
f2	CV	4	1	18	14	168	0.421	0.347	-198.76860094	-199.46630985	-199.48861417
f2	CV	5	1	18	14	290	2.777	2.205	-198.77298571	-199.48790184	-199.51115611
f2	FC	2	1	18	14	36	0.004	0.004	-198.68616632	-199.10442428	-199.11444235
f2	FC	3	1	18	14	86	0.034	0.031	-198.75273797	-199.29161413	-199.31043135
f2	FC	4	1	18	14	168	0.308	0.271	-198.76860094	-199.34396848	-199.36523040
f2	FC	5	1	18	14	290	2.077	1.8	-198.77298571	-199.36170130	-199.38387699
f2co	CV	2	1	32	24	72	0.061	0.05	-311.63481755	-312.46166235	-312.48122846
f2co	CV	3	1	32	24	172	0.962	0.618	-311.73865810	-312.84086490	-312.87595886
f2co	CV	4	1	32	24	336	12.149	6.802	-311.76256462	-312.94722149	-312.98614998
f2co	CV	5	1	32	24	580	119.631	74.674	-311.76863532	-312.98127495	-313.02154491
f2co	FC	2	1	32	24	72	0.033	0.028	-311.63481755	-312.33888981	-312.35778558
f2co	FC	3	1	32	24	172	0.578	0.428	-311.73865810	-312.63081150	-312.66431937
f2co	FC	4	1	32	24	336	7.717	5.423	-311.76256462	-312.71235153	-312.74943839
f2co	FC	5	1	32	24	580	83.211	63.994	-311.76863532	-312.73914829	-312.77751273
fccf	CV	2	1	30	22	72	0.058	0.048	-274.47873450	-275.24749307	-275.26802161
fccf	CV	3	1	30	22	172	0.932	0.62	-274.56842984	-275.58402364	-275.61863669
fccf	CV	4	1	30	22	336	9.506	5.281	-274.58887931	-275.67821172	-275.71609606
fccf	CV	5	1	30	22	580	340.656	300.335	-274.59426586	-275.70819657	-275.74721468
fccf	FC	2	1	30	22	72	0.032	0.028	-274.47873450	-275.12501427	-275.14479698
fccf	FC	3	1	30	22	172	0.568	0.441	-274.56842984	-275.37781469	-275.41073417

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
fccf	FC	4	1	30	22	336	5.979	4.307	-274.58887931	-275.44780413	-275.48373638
fccf	FC	5	1	30	22	580	151.67	135.647	-274.59426586	-275.47073768	-275.50773976
formic	CV	2	1	24	18	64	0.031	0.027	-188.78270782	-189.39918345	-189.41612977
formic	CV	3	1	24	18	157	0.54	0.417	-188.84223441	-189.64022768	-189.66865315
formic	CV	4	1	24	18	312	5.438	3.845	-188.85638369	-189.70780858	-189.73890770
formic	CV	5	1	24	18	545	268.693	251.465	-188.85981427	-189.72882200	-189.76083205
formic	FC	2	1	24	18	64	0.019	0.017	-188.78270782	-189.30761026	-189.32400619
formic	FC	3	1	24	18	157	0.348	0.296	-188.84223441	-189.48725426	-189.51442296
formic	FC	4	1	24	18	312	3.613	2.927	-188.85638369	-189.53703134	-189.56668250
formic	FC	5	1	24	18	545	205.733	198.387	-188.85981427	-189.55285452	-189.58336946
h2cn	CV	2	2	15	11	46	0.028	0.024	-93.44159502	-93.79137745	-93.80156569
h2cn	CV	3	2	15	11	114	1.034	0.966	-93.46678875	-93.91122795	-93.92730496
h2cn	CV	4	2	15	11	228	16.869	15.924	-93.47286484	-93.94399800	-93.96142414
h2cn	CV	5	2	15	11	400	226.739	218.729	-93.47424835	-93.95377266	-93.97164650
h2cn	FC	2	2	15	11	46	0.021	0.019	-93.44159502	-93.73094996	-93.74072841
h2cn	FC	3	2	15	11	114	0.969	0.931	-93.46678875	-93.81330944	-93.82851173
h2cn	FC	4	2	15	11	228	16.356	15.916	-93.47286484	-93.83482832	-93.85125719
h2cn	FC	5	2	15	11	400	223.23	219.713	-93.47424835	-93.84137406	-93.85822161
h2co	CV	2	1	16	12	46	0.008	0.007	-113.87673443	-114.27762717	-114.28872966
h2co	CV	3	1	16	12	114	0.103	0.092	-113.91231152	-114.42438340	-114.44241344
h2co	CV	4	1	16	12	228	1.042	0.861	-113.92083610	-114.46525391	-114.48486843
h2co	CV	5	1	16	12	400	35.871	34.395	-113.92290844	-114.47779510	-114.49794121
h2co	FC	2	1	16	12	46	0.005	0.005	-113.87673443	-114.21692407	-114.22762978
h2co	FC	3	1	16	12	114	0.072	0.066	-113.91231152	-114.32408202	-114.34123665
h2co	FC	4	1	16	12	228	0.789	0.71	-113.92083610	-114.35331615	-114.37192824
h2co	FC	5	1	16	12	400	22.987	22.353	-113.92290844	-114.36247337	-114.38158611
h2o	CV	2	1	10	8	28	0.002	0.002	-76.02709961	-76.27470052	-76.27834035
h2o	CV	3	1	10	8	71	0.013	0.012	-76.05720230	-76.38174526	-76.39011097
h2o	CV	4	1	10	8	144	0.147	0.139	-76.06482317	-76.41154498	-76.42112412
h2o	CV	5	1	10	8	255	1.209	1.131	-76.06701628	-76.42105304	-76.43108083
h2o	FC	2	1	10	8	28	0.001	0.001	-76.02709961	-76.24387407	-76.24736385
h2o	FC	3	1	10	8	71	0.01	0.01	-76.05720230	-76.32901652	-76.33702037
h2o	FC	4	1	10	8	144	0.127	0.122	-76.06482317	-76.35263424	-76.36178932
h2o	FC	5	1	10	8	255	1.011	0.97	-76.06701628	-76.36033548	-76.36992267

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
h2s	CV	2	1	18	8	37	0.005	0.004	-398.69849904	-399.01916468	-399.02425747
h2s	CV	3	1	18	8	87	0.044	0.038	-398.71552087	-399.22629047	-399.23713040
h2s	CV	4	1	18	8	169	0.391	0.31	-398.71931111	-399.31908778	-399.33186998
h2s	CV	5	1	18	8	291	2.43	1.837	-398.71999409	-399.35732771	-399.37069845
h2s	FC	2	1	18	8	37	0.002	0.002	-398.69849904	-398.86965744	-398.87340914
h2s	FC	3	1	18	8	87	0.017	0.016	-398.71552087	-398.93267805	-398.94092352
h2s	FC	4	1	18	8	169	0.2	0.191	-398.71931111	-398.94925918	-398.95876992
h2s	FC	5	1	18	8	291	1.493	1.433	-398.71999409	-398.95359238	-398.96346208
hccf	CV	2	1	22	16	59	0.02	0.017	-175.65772888	-176.21094611	-176.22739113
hccf	CV	3	1	22	16	143	0.299	0.246	-175.71367450	-176.43241291	-176.45873121
hccf	CV	4	1	22	16	282	3.409	2.486	-175.72594713	-176.49350694	-176.52203867
hccf	CV	5	1	22	16	490	31.307	22.487	-175.72902808	-176.51257164	-176.54184620
hccf	FC	2	1	22	16	59	0.011	0.01	-175.65772888	-176.11959777	-176.13545445
hccf	FC	3	1	22	16	143	0.179	0.158	-175.71367450	-176.28127555	-176.30628971
hccf	FC	4	1	22	16	282	1.937	1.575	-175.72594713	-176.32476871	-176.35180505
hccf	FC	5	1	22	16	490	19.699	16.279	-175.72902808	-176.33871903	-176.36645168
hcl	CV	2	1	18	8	32	0.005	0.004	-460.09159444	-460.41138582	-460.41549367
hcl	CV	3	1	18	8	73	0.025	0.022	-460.10811350	-460.63571086	-460.64640468
hcl	CV	4	1	18	8	139	0.202	0.17	-460.11193755	-460.73314066	-460.74604194
hcl	CV	5	1	18	8	236	1.227	0.933	-460.11259652	-460.77334449	-460.78691254
hcl	FC	2	1	18	8	32	0.001	0.001	-460.09159444	-460.26150170	-460.26442962
hcl	FC	3	1	18	8	73	0.01	0.009	-460.10811350	-460.33509130	-460.34335063
hcl	FC	4	1	18	8	139	0.092	0.088	-460.11193755	-460.35610043	-460.36593590
hcl	FC	5	1	18	8	236	0.67	0.641	-460.11259652	-460.36173564	-460.37202463
hcn	CV	2	1	14	10	41	0.005	0.005	-92.88421938	-93.24438602	-93.25750234
hcn	CV	3	1	14	10	100	0.057	0.052	-92.90867558	-93.36108705	-93.38051959
hcn	CV	4	1	14	10	198	0.536	0.46	-92.91417058	-93.39316473	-93.41391140
hcn	CV	5	1	14	10	345	3.545	3.021	-92.91535676	-93.40283268	-93.42401342
hcn	FC	2	1	14	10	41	0.003	0.003	-92.88421938	-93.18396623	-93.19664523
hcn	FC	3	1	14	10	100	0.04	0.038	-92.90867558	-93.26301036	-93.28149200
hcn	FC	4	1	14	10	198	0.481	0.451	-92.91417058	-93.28377718	-93.30344115
hcn	FC	5	1	14	10	345	3.943	3.746	-92.91535676	-93.29019807	-93.31026472
hcnh	CV	2	2	15	11	46	0.028	0.024	-93.41076423	-93.77359352	-93.78531173
hcnh	CV	3	2	15	11	114	0.981	0.913	-93.43762733	-93.89584288	-93.91392291

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
hcnh	CV	4	2	15	11	228	16.88	15.935	-93.44417648	-93.92960320	-93.94911217
hcnh	CV	5	2	15	11	400	224.53	216.569	-93.44575919	-93.93979754	-93.95978751
hcnh	FC	2	2	15	11	46	0.022	0.02	-93.41076423	-93.71310754	-93.72441768
hcnh	FC	3	2	15	11	114	0.921	0.884	-93.43762733	-93.79787470	-93.81507397
hcnh	FC	4	2	15	11	228	15.474	15.031	-93.44417648	-93.82038196	-93.83888732
hcnh	FC	5	2	15	11	400	222.445	218.93	-93.44575919	-93.82734876	-93.84630604
hcnno	CV	2	1	22	16	59	0.022	0.019	-167.64476919	-168.23799763	-168.26213557
hcnno	CV	3	1	22	16	143	0.333	0.28	-167.69519636	-168.44953504	-168.48482217
hcnno	CV	4	1	22	16	282	3.602	2.675	-167.70697827	-168.50876697	-168.54654114
hcnno	CV	5	1	22	16	490	34.445	25.593	-167.70986261	-168.52706471	-168.56567989
hcnno	FC	2	1	22	16	59	0.012	0.011	-167.64476919	-168.14638226	-168.16986808
hcnno	FC	3	1	22	16	143	0.203	0.182	-167.69519636	-168.29849299	-168.33233584
hcnno	FC	4	1	22	16	282	2.059	1.695	-167.70697827	-168.34025897	-168.37638263
hcnno	FC	5	1	22	16	490	20.763	17.32	-167.70986261	-168.35350768	-168.39042214
hco	CV	2	2	15	11	41	0.018	0.016	-113.25935573	-113.63446835	-113.64609899
hco	CV	3	2	15	11	100	0.58	0.54	-113.29324073	-113.77420412	-113.79266208
hco	CV	4	2	15	11	198	9.198	8.614	-113.30151459	-113.81351867	-113.83351299
hco	CV	5	2	15	11	345	116.429	111.595	-113.30347967	-113.82562745	-113.84614315
hco	FC	2	2	15	11	41	0.014	0.013	-113.25935573	-113.57402265	-113.58527415
hco	FC	3	2	15	11	100	0.532	0.509	-113.29324073	-113.67412124	-113.69172068
hco	FC	4	2	15	11	198	8.815	8.533	-113.30151459	-113.70179695	-113.72080647
hco	FC	5	2	15	11	345	114.852	112.743	-113.30347967	-113.71052271	-113.73002288
hf	CV	2	1	10	8	23	0.001	0.001	-100.01957043	-100.26530501	-100.26781083
hf	CV	3	1	10	8	57	0.006	0.006	-100.05809030	-100.39348710	-100.40057515
hf	CV	4	1	10	8	114	0.059	0.056	-100.06771445	-100.42983280	-100.43824519
hf	CV	5	1	10	8	200	0.496	0.465	-100.07042315	-100.44163931	-100.45055090
hf	FC	2	1	10	8	23	0.001	0.001	-100.01957043	-100.23424979	-100.23663197
hf	FC	3	1	10	8	57	0.005	0.005	-100.05809030	-100.33844012	-100.34520494
hf	FC	4	1	10	8	114	0.052	0.05	-100.06771445	-100.36818037	-100.37620737
hf	FC	5	1	10	8	200	0.382	0.366	-100.07042315	-100.37804771	-100.38655739
hnc	CV	2	1	14	10	41	0.005	0.005	-92.86704566	-93.21979823	-93.23236135
hnc	CV	3	1	14	10	100	0.06	0.055	-92.89293638	-93.33765847	-93.35637714
hnc	CV	4	1	14	10	198	0.567	0.491	-92.89866508	-93.36982462	-93.38986804
hnc	CV	5	1	14	10	345	3.756	3.234	-92.89991900	-93.37947382	-93.39995672

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
hnc	FC	2	1	14	10	41	0.003	0.003	-92.86704566	-93.15944347	-93.17160287
hnc	FC	3	1	14	10	100	0.043	0.041	-92.89293638	-93.23981761	-93.25764538
hnc	FC	4	1	14	10	198	0.51	0.481	-92.89866508	-93.26070883	-93.27973694
hnc	FC	5	1	14	10	345	3.935	3.736	-92.89991900	-93.26712219	-93.28656045
hnco	CV	2	1	22	16	59	0.021	0.019	-167.77970556	-168.35306401	-168.37370449
hnco	CV	3	1	22	16	143	0.337	0.282	-167.83019260	-168.56543205	-168.59649049
hnco	CV	4	1	22	16	282	3.803	2.844	-167.84199967	-168.62490629	-168.65833234
hnco	CV	5	1	22	16	490	34.54	25.546	-167.84470380	-168.64314922	-168.67737477
hnco	FC	2	1	22	16	59	0.012	0.011	-167.77970556	-168.26155675	-168.28161737
hnco	FC	3	1	22	16	143	0.202	0.18	-167.83019260	-168.41446564	-168.44421569
hnco	FC	4	1	22	16	282	2.161	1.781	-167.84199967	-168.45645447	-168.48837838
hnco	FC	5	1	22	16	490	21.951	18.43	-167.84470380	-168.46964206	-168.50231842
hnnn	CV	2	1	22	16	59	0.023	0.02	-163.85612333	-164.46048711	-164.48597171
hnnn	CV	3	1	22	16	143	0.356	0.3	-163.90360047	-164.66483187	-164.70160098
hnnn	CV	4	1	22	16	282	3.961	2.999	-163.91454413	-164.72145357	-164.76072437
hnnn	CV	5	1	22	16	490	36.244	27.239	-163.91714821	-164.73883619	-164.77896735
hnnn	FC	2	1	22	16	59	0.013	0.012	-163.85612333	-164.36893744	-164.39376324
hnnn	FC	3	1	22	16	143	0.204	0.182	-163.90360047	-164.51432284	-164.54963634
hnnn	FC	4	1	22	16	282	2.304	1.926	-163.91454413	-164.55360405	-164.59121436
hnnn	FC	5	1	22	16	490	23.187	19.692	-163.91714821	-164.56603384	-164.60445548
hno	CV	2	1	16	12	41	0.007	0.006	-129.79859830	-130.22983367	-130.24312901
hno	CV	3	1	16	12	100	0.073	0.066	-129.83693568	-130.38848642	-130.40996167
hno	CV	4	1	16	12	198	0.667	0.554	-129.84680617	-130.43336514	-130.45673914
hno	CV	5	1	16	12	345	4.604	3.8	-129.84926223	-130.44740545	-130.47145361
hno	FC	2	1	16	12	41	0.005	0.004	-129.79859830	-130.16899838	-130.18185837
hno	FC	3	1	16	12	100	0.052	0.048	-129.83693568	-130.28633548	-130.30684948
hno	FC	4	1	16	12	198	0.548	0.499	-129.84680617	-130.31932020	-130.34159730
hno	FC	5	1	16	12	345	4.112	3.761	-129.84926223	-130.32992018	-130.35283828
hocl	CV	2	1	26	14	50	0.019	0.016	-534.87646793	-535.41700870	-535.42738033
hocl	CV	3	1	26	14	116	0.241	0.201	-534.92190370	-535.74022293	-535.76217368
hocl	CV	4	1	26	14	223	2.08	1.417	-534.93201648	-535.86444475	-535.88988455
hocl	CV	5	1	26	14	381	14.426	9.719	-534.93431188	-535.91352126	-535.94010294
hocl	FC	2	1	26	14	50	0.006	0.006	-534.87646793	-535.23662264	-535.24551400
hocl	FC	3	1	26	14	116	0.09	0.083	-534.92190370	-535.38748208	-535.40639806

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
hocl	FC	4	1	26	14	223	0.791	0.681	-534.93201648	-535.42920324	-535.45089192
hocl	FC	5	1	26	14	381	6.083	5.316	-534.93431188	-535.44194209	-535.46453542
hocn	CV	2	1	22	16	59	0.022	0.019	-167.74146899	-168.31791039	-168.33662001
hocn	CV	3	1	22	16	143	0.317	0.263	-167.79082824	-168.52890547	-168.55842264
hocn	CV	4	1	22	16	282	3.628	2.668	-167.80227141	-168.58761351	-168.61947943
hocn	CV	5	1	22	16	490	32.973	23.961	-167.80490885	-168.60563601	-168.63829036
hocn	FC	2	1	22	16	59	0.012	0.011	-167.74146899	-168.22657099	-168.24467595
hocn	FC	3	1	22	16	143	0.179	0.157	-167.79082824	-168.37811430	-168.40628121
hocn	FC	4	1	22	16	282	2.074	1.697	-167.80227141	-168.41935204	-168.44967184
hocn	FC	5	1	22	16	490	20.778	17.287	-167.80490885	-168.43232303	-168.46338382
hof	CV	2	1	18	14	41	0.008	0.007	-174.74540843	-175.21832296	-175.22854863
hof	CV	3	1	18	14	100	0.091	0.082	-174.80461298	-175.43460023	-175.45421716
hof	CV	4	1	18	14	198	0.837	0.682	-174.81859709	-175.49454421	-175.51664866
hof	CV	5	1	18	14	345	6.046	5.002	-174.82241761	-175.51410163	-175.53711441
hof	FC	2	1	18	14	41	0.005	0.005	-174.74540843	-175.15695502	-175.16680670
hof	FC	3	1	18	14	100	0.064	0.059	-174.80461298	-175.32761903	-175.34636912
hof	FC	4	1	18	14	198	0.615	0.54	-174.81859709	-175.37484463	-175.39594531
hof	FC	5	1	18	14	345	4.532	4.023	-174.82241761	-175.39067507	-175.41264875
honc	CV	2	1	22	16	59	0.021	0.019	-167.64652840	-168.22482406	-168.24400274
honc	CV	3	1	22	16	143	0.334	0.281	-167.69557753	-168.43376819	-168.46391614
honc	CV	4	1	22	16	282	3.764	2.809	-167.70670971	-168.49159808	-168.52417740
honc	CV	5	1	22	16	490	34.522	25.487	-167.70931421	-168.50938284	-168.54278447
honc	FC	2	1	22	16	59	0.012	0.011	-167.64652840	-168.13379296	-168.15236117
honc	FC	3	1	22	16	143	0.205	0.182	-167.69557753	-168.28357858	-168.31235798
honc	FC	4	1	22	16	282	2.203	1.824	-167.70670971	-168.32401056	-168.35502571
honc	FC	5	1	22	16	490	21.954	18.433	-167.70931421	-168.33676483	-168.36855502
hoo	CV	2	2	17	13	41	0.02	0.017	-150.18817990	-150.62275759	-150.63261287
hoo	CV	3	2	17	13	100	0.585	0.534	-150.23723627	-150.80955006	-150.82817113
hoo	CV	4	2	17	13	198	9.266	8.495	-150.24895183	-150.86115943	-150.88198682
hoo	CV	5	2	17	13	345	104.494	98.229	-150.25203341	-150.87761735	-150.89923763
hoo	FC	2	2	17	13	41	0.015	0.013	-150.18817990	-150.56173392	-150.57122938
hoo	FC	3	2	17	13	100	0.535	0.505	-150.23723627	-150.70495837	-150.72273247
hoo	FC	4	2	17	13	198	8.841	8.443	-150.24895183	-150.74428445	-150.76413266
hoo	FC	5	2	17	13	345	109.124	106.044	-150.25203341	-150.75714858	-150.77775680

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
hooh	CV	2	1	18	14	46	0.009	0.009	-150.78486673	-151.25755010	-151.26804920
hooh	CV	3	1	18	14	114	0.135	0.12	-150.83651146	-151.45409727	-151.47415205
hooh	CV	4	1	18	14	228	1.303	1.027	-150.84853298	-151.50799917	-151.53040970
hooh	CV	5	1	18	14	400	9.961	7.703	-150.85173426	-151.52526890	-151.54852442
hooh	FC	2	1	18	14	46	0.006	0.006	-150.78486673	-151.19632569	-151.20644789
hooh	FC	3	1	18	14	114	0.096	0.088	-150.83651146	-151.34932916	-151.36851013
hooh	FC	4	1	18	14	228	0.948	0.814	-150.84853298	-151.39093476	-151.41233545
hooh	FC	5	1	18	14	400	7.301	6.211	-150.85173426	-151.40460824	-151.42681868
hs	CV	2	2	17	7	32	0.008	0.006	-398.09119821	-398.37840741	-398.38221956
hs	CV	3	2	17	7	73	0.141	0.122	-398.10649618	-398.57837952	-398.58734665
hs	CV	4	2	17	7	139	1.855	1.683	-398.11007778	-398.66898326	-398.67972458
hs	CV	5	2	17	7	236	15.717	14.222	-398.11068097	-398.70661746	-398.71788942
hs	FC	2	2	17	7	32	0.004	0.004	-398.09119821	-398.22898835	-398.23155544
hs	FC	3	2	17	7	73	0.099	0.095	-398.10649618	-398.28502933	-398.29150112
hs	FC	4	2	17	7	139	1.557	1.523	-398.11007778	-398.29940397	-398.30697858
hs	FC	5	2	17	7	236	13.702	13.501	-398.11068097	-398.30312609	-398.31100384
ketene	CV	2	1	22	16	64	0.028	0.025	-151.74128554	-152.29451512	-152.31326609
ketene	CV	3	1	22	16	157	0.465	0.37	-151.78548188	-152.49001076	-152.51846030
ketene	CV	4	1	22	16	312	5.088	3.733	-151.79562551	-152.54416093	-152.57475752
ketene	CV	5	1	22	16	545	53.842	40.083	-151.79795599	-152.56056378	-152.59186047
ketene	FC	2	1	22	16	64	0.016	0.015	-151.74128554	-152.20344024	-152.22159840
ketene	FC	3	1	22	16	157	0.263	0.225	-151.78548188	-152.34132682	-152.36847637
ketene	FC	4	1	22	16	312	2.935	2.403	-151.79562551	-152.37831971	-152.40742788
ketene	FC	5	1	22	16	545	32.242	26.904	-151.79795599	-152.38974354	-152.41950646
methanol	CV	2	1	18	14	56	0.015	0.013	-115.04994684	-115.48168833	-115.49046052
methanol	CV	3	1	18	14	142	0.222	0.185	-115.08985356	-115.64306150	-115.65912801
methanol	CV	4	1	18	14	288	2.74	2.13	-115.09905296	-115.68703366	-115.70482796
methanol	CV	5	1	18	14	510	28.476	22.321	-115.10150732	-115.70061202	-115.71898645
methanol	FC	2	1	18	14	56	0.009	0.008	-115.04994684	-115.42060906	-115.42903416
methanol	FC	3	1	18	14	142	0.164	0.146	-115.08985356	-115.54243718	-115.55772731
methanol	FC	4	1	18	14	288	2.011	1.714	-115.09905296	-115.57478731	-115.59168483
methanol	FC	5	1	18	14	510	21.906	18.997	-115.10150732	-115.58498673	-115.60243455
n2	CV	2	1	14	10	36	0.004	0.003	-108.95469995	-109.33277194	-109.34596562
n2	CV	3	1	14	10	86	0.032	0.029	-108.98410388	-109.46252568	-109.48266166

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
n2	CV	4	1	14	10	168	0.277	0.239	-108.99094690	-109.49824894	-109.51983428
n2	CV	5	1	14	10	290	1.857	1.57	-108.99250225	-109.50933691	-109.53142448
n2	FC	2	1	14	10	36	0.002	0.002	-108.95469995	-109.27222578	-109.28499101
n2	FC	3	1	14	10	86	0.026	0.025	-108.98410388	-109.36252288	-109.38170159
n2	FC	4	1	14	10	168	0.244	0.228	-108.99094690	-109.38665665	-109.40714845
n2	FC	5	1	14	10	290	1.81	1.701	-108.99250225	-109.39443505	-109.41539616
n2h	CV	2	2	15	11	41	0.019	0.017	-109.43853948	-109.82036564	-109.83246610
n2h	CV	3	2	15	11	100	0.609	0.569	-109.46843392	-109.95446391	-109.97370055
n2h	CV	4	2	15	11	198	9.681	9.087	-109.47607444	-109.99192933	-110.01278762
n2h	CV	5	2	15	11	345	109.701	104.949	-109.47791043	-110.00346462	-110.02489331
n2h	FC	2	2	15	11	41	0.015	0.013	-109.43853948	-109.75962255	-109.77130468
n2h	FC	3	2	15	11	100	0.528	0.506	-109.46843392	-109.85440097	-109.87271442
n2h	FC	4	2	15	11	198	9.297	9.015	-109.47607444	-109.88031563	-109.90012003
n2h	FC	5	2	15	11	345	108.184	106.052	-109.47791043	-109.88855386	-109.90889742
n2h4	CV	2	1	18	14	56	0.014	0.013	-111.18743189	-111.63093013	-111.64076778
n2h4	CV	3	1	18	14	142	0.234	0.198	-111.22481877	-111.78885326	-111.80659335
n2h4	CV	4	1	18	14	288	2.754	2.144	-111.23370929	-111.83195393	-111.85154225
n2h4	CV	5	1	18	14	510	28.472	22.322	-111.23614990	-111.84528879	-111.86552053
n2h4	FC	2	1	18	14	56	0.009	0.008	-111.18743189	-111.56946307	-111.57893910
n2h4	FC	3	1	18	14	142	0.174	0.156	-111.22481877	-111.68810921	-111.70503793
n2h4	FC	4	1	18	14	288	2.021	1.725	-111.23370929	-111.71965304	-111.73830688
n2h4	FC	5	1	18	14	510	21.954	19.018	-111.23614990	-111.72969073	-111.74895752
n2o	CV	2	1	22	16	54	0.019	0.017	-183.69644357	-184.31435516	-184.34054288
n2o	CV	3	1	22	16	129	0.234	0.197	-183.75045452	-184.53601172	-184.57394939
n2o	CV	4	1	22	16	252	2.391	1.774	-183.76286629	-184.59790815	-184.63848107
n2o	CV	5	1	22	16	435	17.022	12.072	-183.76577025	-184.61710773	-184.65858485
n2o	FC	2	1	22	16	54	0.01	0.01	-183.69644357	-184.22277725	-184.24831253
n2o	FC	3	1	22	16	129	0.143	0.127	-183.75045452	-184.38336181	-184.41983356
n2o	FC	4	1	22	16	252	1.385	1.142	-183.76286629	-184.42754430	-184.46644152
n2o	FC	5	1	22	16	435	10.333	8.394	-183.76577025	-184.44163789	-184.48138840
nccn	CV	2	1	26	18	72	0.053	0.046	-184.60515939	-185.29951095	-185.32895605
nccn	CV	3	1	26	18	172	0.817	0.602	-184.64945196	-185.52287967	-185.56512043
nccn	CV	4	1	26	18	336	8.53	5.685	-184.65955806	-185.58488414	-185.62977203
nccn	CV	5	1	26	18	580	81.79	53.103	-184.66169514	-185.60355527	-185.64932085

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
nccn	FC	2	1	26	18	72	0.027	0.024	-184.60515939	-185.17845794	-185.20699904
nccn	FC	3	1	26	18	172	0.449	0.375	-184.64945196	-185.32666238	-185.36695628
nccn	FC	4	1	26	18	336	4.74	3.778	-184.65955806	-185.36607683	-185.40875089
nccn	FC	5	1	26	18	580	47.754	38.127	-184.66169514	-185.37825944	-185.42174714
nh	CV	2	3	8	6	23	0.003	0.003	-54.96678733	-55.12392871	-55.12574741
nh	CV	3	3	8	6	57	0.049	0.046	-54.98135995	-55.18943047	-55.19370728
nh	CV	4	3	8	6	114	0.838	0.814	-54.98516282	-55.20659643	-55.21150324
nh	CV	5	3	8	6	200	8.556	8.4	-54.98616465	-55.21176113	-55.21687654
nh	FC	2	3	8	6	23	0.003	0.002	-54.96678733	-55.09383012	-55.09552122
nh	FC	3	3	8	6	57	0.045	0.043	-54.98135995	-55.13974186	-55.14371136
nh	FC	4	3	8	6	114	0.784	0.769	-54.98516282	-55.15115953	-55.15570812
nh	FC	5	3	8	6	200	8.121	8.028	-54.98616465	-55.15468506	-55.15943012
nh2	CV	2	2	9	7	28	0.004	0.004	-55.56753183	-55.76449416	-55.76753015
nh2	CV	3	2	9	7	71	0.118	0.112	-55.58616808	-55.84086695	-55.84707214
nh2	CV	4	2	9	7	144	2.044	1.984	-55.59070168	-55.86114273	-55.86814667
nh2	CV	5	2	9	7	255	21.672	21.199	-55.59197549	-55.86736260	-55.87464467
nh2	FC	2	2	9	7	28	0.004	0.004	-55.56753183	-55.73408663	-55.73697053
nh2	FC	3	2	9	7	71	0.111	0.107	-55.58616808	-55.79085034	-55.79670594
nh2	FC	4	2	9	7	144	1.978	1.938	-55.59070168	-55.80535679	-55.81195535
nh2	FC	5	2	9	7	255	21.666	21.381	-55.59197549	-55.80993190	-55.81679470
nh2cl	CV	2	1	26	14	55	0.024	0.021	-515.07554218	-515.60322242	-515.61373433
nh2cl	CV	3	1	26	14	130	0.313	0.248	-515.11109662	-515.90384958	-515.92517887
nh2cl	CV	4	1	26	14	253	3.297	2.242	-515.11879500	-516.02177451	-516.04634388
nh2cl	CV	5	1	26	14	436	24.387	15.238	-515.12047116	-516.06860068	-516.09421478
nh2cl	FC	2	1	26	14	55	0.008	0.007	-515.07554218	-515.42280735	-515.43185953
nh2cl	FC	3	1	26	14	130	0.129	0.118	-515.11109662	-515.55324617	-515.57157886
nh2cl	FC	4	1	26	14	253	1.29	1.117	-515.11879500	-515.58905106	-515.60991482
nh2cl	FC	5	1	26	14	436	9.794	8.33	-515.12047116	-515.59968636	-515.62136047
nh3	CV	2	1	10	8	33	0.002	0.002	-56.19628184	-56.43312912	-56.43743168
nh3	CV	3	1	10	8	85	0.022	0.021	-56.21806819	-56.51892417	-56.52719313
nh3	CV	4	1	10	8	174	0.314	0.294	-56.22315396	-56.54169318	-56.55092162
nh3	CV	5	1	10	8	310	2.577	2.423	-56.22471044	-56.54879934	-56.55836084
nh3	FC	2	1	10	8	33	0.002	0.002	-56.19628184	-56.40232098	-56.40645803
nh3	FC	3	1	10	8	85	0.019	0.018	-56.21806819	-56.46841580	-56.47631410

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
nh3	FC	4	1	10	8	174	0.234	0.224	-56.22315396	-56.48538251	-56.49418212
nh3	FC	5	1	10	8	310	2.116	2.034	-56.22471044	-56.49083489	-56.49995310
no	CV	2	2	15	11	36	0.012	0.01	-129.26064587	-129.65748401	-129.66987554
no	CV	3	2	15	11	86	0.302	0.276	-129.29706368	-129.80857089	-129.82862547
no	CV	4	2	15	11	168	4.389	4.108	-129.30640634	-129.85121992	-129.87302075
no	CV	5	2	15	11	290	49.762	47.021	-129.30859489	-129.86449979	-129.88691337
no	FC	2	2	15	11	36	0.009	0.008	-129.26064587	-129.59677553	-129.60876832
no	FC	3	2	15	11	86	0.268	0.254	-129.29706368	-129.70642756	-129.72557436
no	FC	4	2	15	11	168	4.182	4.04	-129.30640634	-129.73716285	-129.75792209
no	FC	5	2	15	11	290	48.233	47.039	-129.30859489	-129.74699716	-129.76833654
no2	CV	2	2	23	17	54	0.059	0.046	-204.04866295	-204.68732663	-204.71317983
no2	CV	3	2	23	17	129	1.82	1.577	-204.11065286	-204.93165900	-204.97008972
no2	CV	4	2	23	17	252	26.819	22.425	-204.12603822	-205.00116088	-205.04258829
no2	CV	5	2	23	17	435	341.037	305.162	-204.12965669	-205.02290669	-205.06539646
no2	FC	2	2	23	17	54	0.04	0.034	-204.04866295	-204.59579589	-204.62103841
no2	FC	3	2	23	17	129	1.535	1.417	-204.11065286	-204.77699592	-204.81402736
no2	FC	4	2	23	17	252	23.102	21.225	-204.12603822	-204.82845770	-204.86827741
no2	FC	5	2	23	17	435	307.133	292.451	-204.12965669	-204.84496261	-204.88579333
o2	CV	2	3	16	12	36	0.01	0.008	-149.62845140	-150.04859551	-150.05960042
o2	CV	3	3	16	12	86	0.26	0.232	-149.67594295	-150.22524647	-150.24464795
o2	CV	4	3	16	12	168	3.861	3.521	-149.68778107	-150.27456531	-150.29599157
o2	CV	5	3	16	12	290	40.665	37.346	-149.69078755	-150.29014142	-150.31228833
o2	FC	2	3	16	12	36	0.007	0.006	-149.62845140	-149.98772887	-149.99837312
o2	FC	3	3	16	12	86	0.227	0.211	-149.67594295	-150.12072989	-150.13928732
o2	FC	4	3	16	12	168	3.517	3.345	-149.68778107	-150.15776330	-150.17821330
o2	FC	5	3	16	12	290	38.399	36.892	-149.69078755	-150.16974252	-150.19088065
ocs	CV	2	1	30	16	63	0.035	0.03	-510.29553122	-510.95898935	-510.98230889
ocs	CV	3	1	30	16	145	0.547	0.399	-510.34292372	-511.29419513	-511.33014856
ocs	CV	4	1	30	16	277	4.945	2.922	-510.35372952	-511.42373471	-511.46313926
ocs	CV	5	1	30	16	471	37.617	21.919	-510.35591384	-511.47372375	-511.51425259
ocs	FC	2	1	30	16	63	0.011	0.01	-510.29553122	-510.74887171	-510.77036090
ocs	FC	3	1	30	16	145	0.19	0.167	-510.34292372	-510.90034306	-510.93267304
ocs	FC	4	1	30	16	277	1.819	1.5	-510.35372952	-510.94201652	-510.97697638
ocs	FC	5	1	30	16	471	17.596	15.125	-510.35591384	-510.95470420	-510.99052117

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
oh	CV	2	2	9	7	23	0.003	0.003	-75.39405456	-75.59387935	-75.59604938
oh	CV	3	2	9	7	57	0.046	0.042	-75.41935241	-75.68954723	-75.69525631
oh	CV	4	2	9	7	114	0.806	0.777	-75.42592785	-75.71589075	-75.72258626
oh	CV	5	2	9	7	200	7.682	7.494	-75.42773139	-75.72418701	-75.73123636
oh	FC	2	2	9	7	23	0.003	0.002	-75.39405456	-75.56338152	-75.56542078
oh	FC	3	2	9	7	57	0.043	0.04	-75.41935241	-75.63717955	-75.64256108
oh	FC	4	2	9	7	114	0.783	0.764	-75.42592785	-75.65736249	-75.66367226
oh	FC	5	2	9	7	200	7.527	7.408	-75.42773139	-75.66385821	-75.67050686
oxirene	CV	2	1	22	16	64	0.026	0.023	-151.59525708	-152.15917485	-152.17871773
oxirene	CV	3	1	22	16	157	0.46	0.365	-151.64359005	-152.36136421	-152.39152463
oxirene	CV	4	1	22	16	312	5.106	3.752	-151.65455928	-152.41699777	-152.44958663
oxirene	CV	5	1	22	16	545	51.18	37.422	-151.65751992	-152.43452824	-152.46796477
oxirene	FC	2	1	22	16	64	0.016	0.014	-151.59525708	-152.06835421	-152.08723817
oxirene	FC	3	1	22	16	157	0.262	0.223	-151.64359005	-152.21322485	-152.24195787
oxirene	FC	4	1	22	16	312	2.886	2.352	-151.65455928	-152.25180108	-152.28276397
oxirene	FC	5	1	22	16	545	32.527	27.142	-151.65751992	-152.26438866	-152.29615070
p2	CV	2	1	30	10	54	0.026	0.022	-681.47117064	-682.01564756	-682.03420002
p2	CV	3	1	30	10	118	0.265	0.205	-681.49309145	-682.36872525	-682.39736758
p2	CV	4	1	30	10	218	2.061	1.186	-681.49867435	-682.53732551	-682.56931885
p2	CV	5	1	30	10	362	52.487	46.823	-681.49950122	-682.60928295	-682.64237924
p2	FC	2	1	30	10	54	0.004	0.003	-681.47117064	-681.72028779	-681.73528910
p2	FC	3	1	30	10	118	0.057	0.054	-681.49309145	-681.79168181	-681.81392857
p2	FC	4	1	30	10	218	0.59	0.553	-681.49867435	-681.81222908	-681.83632827
p2	FC	5	1	30	10	362	26.127	25.896	-681.49950122	-681.81794970	-681.84264426
ph3	CV	2	1	18	8	42	0.007	0.006	-342.47541533	-342.78858008	-342.79387354
ph3	CV	3	1	18	8	101	0.073	0.063	-342.49071445	-342.97936685	-342.98889822
ph3	CV	4	1	18	8	199	0.713	0.545	-342.49409962	-343.06604316	-343.07715424
ph3	CV	5	1	18	8	346	4.965	3.777	-342.49468276	-343.10230974	-343.11391382
ph3	FC	2	1	18	8	42	0.002	0.002	-342.47541533	-342.64071383	-342.64454144
ph3	FC	3	1	18	8	101	0.028	0.027	-342.49071445	-342.69032401	-342.69713489
ph3	FC	4	1	18	8	199	0.348	0.332	-342.49409962	-342.70298830	-342.71065908
ph3	FC	5	1	18	8	346	3.055	2.939	-342.49468276	-342.70615351	-342.71407028
s2	CV	2	3	32	12	54	0.068	0.041	-795.06802581	-795.63501922	-795.64867405
s2	CV	3	3	32	12	118	1.334	0.962	-795.10124372	-796.03210960	-796.05764576

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
s2	CV	4	3	32	12	218	16.734	10.88	-795.10827566	-796.21399779	-796.24358639
s2	CV	5	3	32	12	362	173.721	125.673	-795.10930328	-796.29002748	-796.32090261
s2	FC	2	3	32	12	54	0.018	0.015	-795.06802581	-795.33633086	-795.34712448
s2	FC	3	3	32	12	118	0.629	0.593	-795.10124372	-795.44553912	-795.46556363
s2	FC	4	3	32	12	218	8.905	8.497	-795.10827566	-795.47506059	-795.49775318
s2	FC	5	3	32	12	362	112.655	109.755	-795.10930328	-795.48329352	-795.50680559
sif	CV	2	2	23	11	45	0.03	0.022	-388.36282106	-388.80783892	-388.81529507
sif	CV	3	2	23	11	102	0.669	0.569	-388.41876786	-389.10581115	-389.12050224
sif	CV	4	2	23	11	193	8.855	7.405	-388.43111437	-389.21805184	-389.23519305
sif	CV	5	2	23	11	326	765.908	752.73	-388.43381833	-389.26430183	-389.28228320
sif	FC	2	2	23	11	45	0.014	0.012	-388.36282106	-388.63554165	-388.64135280
sif	FC	3	2	23	11	102	0.466	0.445	-388.41876786	-388.76629736	-388.77776903
sif	FC	4	2	23	11	193	6.889	6.66	-388.43111437	-388.80165951	-388.81472380
sif	FC	5	2	23	11	326	180.406	178.78	-388.43381833	-388.81260583	-388.82621225
sih	CV	2	2	15	5	32	0.007	0.006	-289.43074621	-289.66227482	-289.66558821
sih	CV	3	2	15	5	73	0.139	0.124	-289.43999144	-289.82948842	-289.83549298
sih	CV	4	2	15	5	139	1.907	1.779	-289.44240633	-289.90580211	-289.91296393
sih	CV	5	2	15	5	236	16.431	15.287	-289.44278780	-289.94046301	-289.94799723
sih	FC	2	2	15	5	32	0.004	0.004	-289.43074621	-289.52112982	-289.52288637
sih	FC	3	2	15	5	73	0.108	0.105	-289.43999144	-289.54520534	-289.54828000
sih	FC	4	2	15	5	139	1.678	1.657	-289.44240633	-289.55135936	-289.55480291
sih	FC	5	2	15	5	236	14.945	14.831	-289.44278780	-289.55270178	-289.55623928
sih3f	CV	2	1	26	14	60	0.03	0.026	-390.17026809	-390.66762418	-390.67457089
sih3f	CV	3	1	26	14	144	0.433	0.328	-390.23227881	-390.98411445	-390.99809865
sih3f	CV	4	1	26	14	283	4.371	2.789	-390.24526969	-391.10067336	-391.11709558
sih3f	CV	5	1	26	14	491	42.297	27.837	-390.24801863	-391.14773220	-391.16498383
sih3f	FC	2	1	26	14	60	0.009	0.009	-390.17026809	-390.49664023	-390.50200021
sih3f	FC	3	1	26	14	144	0.169	0.151	-390.23227881	-390.64492166	-390.65591602
sih3f	FC	4	1	26	14	283	1.773	1.51	-390.24526969	-390.68449712	-390.69708743
sih3f	FC	5	1	26	14	491	20.19	17.852	-390.24801863	-390.69627424	-390.70939871
sih4	CV	2	1	18	8	47	0.008	0.007	-291.24823568	-291.53633498	-291.54031975
sih4	CV	3	1	18	8	115	0.111	0.095	-291.26434112	-291.72225118	-291.72876372
sih4	CV	4	1	18	8	229	1.059	0.791	-291.26791819	-291.80338705	-291.81110163
sih4	CV	5	1	18	8	401	7.999	5.842	-291.26850584	-291.83910093	-291.84721036

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
sih4	FC	2	1	18	8	47	0.003	0.003	-291.24823568	-291.39626290	-291.39878119
sih4	FC	3	1	18	8	115	0.043	0.041	-291.26434112	-291.43788546	-291.44174431
sih4	FC	4	1	18	8	229	0.588	0.561	-291.26791819	-291.44871848	-291.45300888
sih4	FC	5	1	18	8	401	5.121	4.916	-291.26850584	-291.45111857	-291.45552874
sio	CV	2	1	22	10	45	0.012	0.011	-363.79796632	-364.25521374	-364.26936846
sio	CV	3	1	22	10	102	0.121	0.104	-363.84439286	-364.52533951	-364.54709762
sio	CV	4	1	22	10	193	0.934	0.71	-363.85270580	-364.62853254	-364.65271800
sio	CV	5	1	22	10	326	5.897	4.36	-363.85456818	-364.67220001	-364.69720455
sio	FC	2	1	22	10	45	0.003	0.003	-363.79796632	-364.08354970	-364.09584146
sio	FC	3	1	22	10	102	0.043	0.041	-363.84439286	-364.18798760	-364.20622085
sio	FC	4	1	22	10	193	0.447	0.424	-363.85270580	-364.21458493	-364.23436690
sio	FC	5	1	22	10	326	3.287	3.13	-363.85456818	-364.22302893	-364.24332437
so	CV	2	3	24	12	45	0.032	0.023	-472.35701042	-472.85020055	-472.86231698
so	CV	3	3	24	12	102	0.697	0.592	-472.40908258	-473.14990807	-473.17206978
so	CV	4	3	24	12	193	9.243	7.722	-472.41909196	-473.26615282	-473.29136006
so	CV	5	3	24	12	326	89.39	74.723	-472.42137887	-473.31259316	-473.33881377
so	FC	2	3	24	12	45	0.013	0.012	-472.35701042	-472.67034385	-472.68091346
so	FC	3	3	24	12	102	0.473	0.448	-472.40908258	-472.80415730	-472.82325406
so	FC	4	3	24	12	193	6.898	6.636	-472.41909196	-472.83799617	-472.85938269
so	FC	5	3	24	12	326	71.968	69.886	-472.42137887	-472.84872849	-472.87087635
so2	CV	2	1	32	18	63	0.051	0.043	-547.20818289	-547.94936622	-547.97302197
so2	CV	3	1	32	18	145	0.617	0.447	-547.30620454	-548.36643020	-548.40487710
so2	CV	4	1	32	18	277	5.703	3.144	-547.32264954	-548.51170022	-548.55441453
so2	CV	5	1	32	18	471	179.978	157.459	-547.32643682	-548.56766809	-548.61183334
so2	FC	2	1	32	18	63	0.016	0.014	-547.20818289	-547.73887185	-547.76062256
so2	FC	3	1	32	18	145	0.234	0.202	-547.30620454	-547.96803291	-548.00272377
so2	FC	4	1	32	18	277	2.286	1.816	-547.32264954	-548.02477483	-548.06287790
so2	FC	5	1	32	18	471	116.894	112.818	-547.32643682	-548.04324961	-548.08252214
ssh	CV	2	2	33	13	59	0.106	0.07	-795.64030195	-796.22380160	-796.23581197
ssh	CV	3	2	33	13	132	2.518	1.932	-795.67410292	-796.62821612	-796.65218750
ssh	CV	4	2	33	13	248	34.67	23.637	-795.68125690	-796.81202984	-796.84009903
ssh	CV	5	2	33	13	417	354.579	268.614	-795.68239313	-796.88850384	-796.91786695
ssh	FC	2	2	33	13	59	0.032	0.029	-795.64030195	-795.92493232	-795.93413708
ssh	FC	3	2	33	13	132	1.283	1.22	-795.67410292	-796.04144717	-796.06000192

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
ssh	FC	4	2	33	13	248	18.964	18.135	-795.68125690	-796.07294522	-796.09422358
ssh	FC	5	2	33	13	417	232.373	226.601	-795.68239313	-796.08163679	-796.10374494
t-hcoh	CV	2	1	16	12	46	0.008	0.007	-113.80067213	-114.19533520	-114.20543568
t-hcoh	CV	3	1	16	12	114	0.111	0.1	-113.83599874	-114.34230316	-114.35930270
t-hcoh	CV	4	1	16	12	228	1.007	0.826	-113.84454407	-114.38301755	-114.40157701
t-hcoh	CV	5	1	16	12	400	7.757	6.281	-113.84674593	-114.39563917	-114.41472774
t-hcoh	FC	2	1	16	12	46	0.005	0.005	-113.80067213	-114.13493531	-114.14465711
t-hcoh	FC	3	1	16	12	114	0.076	0.071	-113.83599874	-114.24255550	-114.25871739
t-hcoh	FC	4	1	16	12	228	0.844	0.765	-113.84454407	-114.27169692	-114.28929820
t-hcoh	FC	5	1	16	12	400	6.772	6.136	-113.84674593	-114.28095403	-114.29905552
t-hono	CV	2	1	24	18	59	0.03	0.026	-204.65786428	-205.31536637	-205.33716294
t-hono	CV	3	1	24	18	143	0.42	0.338	-204.72226548	-205.56813129	-205.60303839
t-hono	CV	4	1	24	18	282	4.106	2.909	-204.73794371	-205.63941518	-205.67740643
t-hono	CV	5	1	24	18	490	46.628	35.463	-204.74177959	-205.66188796	-205.70098269
t-hono	FC	2	1	24	18	59	0.018	0.016	-204.65786428	-205.22390913	-205.24508712
t-hono	FC	3	1	24	18	143	0.273	0.239	-204.72226548	-205.41365887	-205.44715994
t-hono	FC	4	1	24	18	282	2.762	2.248	-204.73794371	-205.46691936	-205.50329865
t-hono	FC	5	1	24	18	490	33.979	29.269	-204.74177959	-205.48415701	-205.52158891
t-n2h2	CV	2	1	16	12	46	0.007	0.007	-110.00728199	-110.42431138	-110.43728149
t-n2h2	CV	3	1	16	12	114	0.103	0.093	-110.03891610	-110.56514981	-110.58564640
t-n2h2	CV	4	1	16	12	228	0.945	0.765	-110.04711970	-110.60460286	-110.62678173
t-n2h2	CV	5	1	16	12	400	7.373	5.895	-110.04925308	-110.61680670	-110.63957690
t-n2h2	FC	2	1	16	12	46	0.005	0.005	-110.00728199	-110.36342652	-110.37596560
t-n2h2	FC	3	1	16	12	114	0.072	0.067	-110.03891610	-110.46507840	-110.48463488
t-n2h2	FC	4	1	16	12	228	0.794	0.715	-110.04711970	-110.49300464	-110.51411278
t-n2h2	FC	5	1	16	12	400	6.362	5.729	-110.04925308	-110.50191824	-110.52358634
Al	CV	2	2	13	3	27	0.004	0.004	-241.87362874	-242.05154303	-242.05398614
Al	CV	3	2	13	3	59	0.056	0.049	-241.87912101	-242.20744179	-242.21179111
Al	CV	4	2	13	3	109	0.681	0.635	-241.88049061	-242.27928482	-242.28464784
Al	CV	5	2	13	3	181	5.333	5.026	-241.88076194	-242.31402314	-242.31974610
Al	FC	2	2	13	3	27	0.002	0.002	-241.87362874	-241.92124005	-241.92195972
Al	FC	3	2	13	3	59	0.038	0.038	-241.87912101	-241.93042903	-241.93159650
Al	FC	4	2	13	3	109	0.543	0.539	-241.88049061	-241.93276575	-241.93405735
Al	FC	5	2	13	3	181	4.526	4.504	-241.88076194	-241.93326058	-241.93457803

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
B	CV	2	2	5	3	18	0.002	0.002	-24.52997268	-24.61766763	-24.61872374
B	CV	3	2	5	3	43	0.015	0.014	-24.53212018	-24.64097392	-24.64277540
B	CV	4	2	5	3	84	0.22	0.214	-24.53298282	-24.64793794	-24.64989311
B	CV	5	2	5	3	145	2.161	2.132	-24.53312788	-24.64988225	-24.65188121
B	FC	2	2	5	3	18	0.002	0.002	-24.52997268	-24.59012334	-24.59095343
B	FC	3	2	5	3	43	0.015	0.014	-24.53212018	-24.59774997	-24.59911482
B	FC	4	2	5	3	84	0.203	0.201	-24.53298282	-24.59967586	-24.60114811
B	FC	5	2	5	3	145	2.03	2.018	-24.53312788	-24.60016908	-24.60167393
C	CV	2	3	6	4	18	0.002	0.002	-37.68658636	-37.79098432	-37.79211960
C	CV	3	3	6	4	43	0.015	0.014	-37.69166033	-37.82684726	-37.82931970
C	CV	4	3	6	4	84	0.211	0.205	-37.69332962	-37.83650598	-37.83928583
C	CV	5	3	6	4	145	1.979	1.943	-37.69368131	-37.83927308	-37.84214181
C	FC	2	3	6	4	18	0.002	0.002	-37.68658636	-37.76197272	-37.76294774
C	FC	3	3	6	4	43	0.014	0.014	-37.69166033	-37.78048427	-37.78262224
C	FC	4	3	6	4	84	0.188	0.184	-37.69332962	-37.78479311	-37.78719432
C	FC	5	3	6	4	145	1.905	1.887	-37.69368131	-37.78601546	-37.78849597
Cl	CV	2	2	17	7	27	0.005	0.003	-459.47154982	-459.75526577	-459.75793110
Cl	CV	3	2	17	7	59	0.056	0.046	-459.48569051	-459.97112605	-459.97951886
Cl	CV	4	2	17	7	109	0.632	0.56	-459.48924081	-460.06582026	-460.07619060
Cl	CV	5	2	17	7	181	5.008	4.485	-459.48977562	-460.10523644	-460.11619870
Cl	FC	2	2	17	7	27	0.003	0.002	-459.47154982	-459.60555930	-459.60715704
Cl	FC	3	2	17	7	59	0.036	0.034	-459.48569051	-459.67081243	-459.67689256
Cl	FC	4	2	17	7	109	0.51	0.494	-459.48924081	-459.68907286	-459.69650501
Cl	FC	5	2	17	7	181	4.243	4.157	-459.48977562	-459.69392110	-459.70173402
F	CV	2	2	9	7	18	0.002	0.002	-99.37531091	-99.56548880	-99.56670982
F	CV	3	2	9	7	43	0.014	0.013	-99.40558305	-99.67816009	-99.68231764
F	CV	4	2	9	7	84	0.21	0.198	-99.41379882	-99.70995972	-99.71506900
F	CV	5	2	9	7	145	1.924	1.86	-99.41605193	-99.72022495	-99.72568156
F	FC	2	2	9	7	18	0.002	0.002	-99.37531091	-99.53472335	-99.53584851
F	FC	3	2	9	7	43	0.013	0.012	-99.40558305	-99.62339863	-99.62728976
F	FC	4	2	9	7	84	0.201	0.193	-99.41379882	-99.64860164	-99.65338981
F	FC	5	2	9	7	145	1.908	1.864	-99.41605193	-99.65693019	-99.66205181
N	CV	2	4	7	5	18	0.002	0.002	-54.39120752	-54.51155452	-54.51235036
N	CV	3	4	7	5	43	0.014	0.013	-54.40080109	-54.56471230	-54.56738385

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
N	CV	4	4	7	5	84	0.199	0.191	-54.40373484	-54.57828008	-54.58143988
N	CV	5	4	7	5	145	1.834	1.791	-54.40444305	-54.58225337	-54.58555929
N	FC	2	4	7	5	18	0.002	0.002	-54.39120752	-54.48169855	-54.48240110
N	FC	3	4	7	5	43	0.012	0.012	-54.40080109	-54.51520331	-54.51763216
N	FC	4	4	7	5	84	0.182	0.178	-54.40373484	-54.52302726	-54.52590094
N	FC	5	4	7	5	145	1.684	1.661	-54.40444305	-54.52536151	-54.52837189
O	CV	2	3	8	6	18	0.002	0.002	-74.79228596	-74.94520131	-74.94619972
O	CV	3	3	8	6	43	0.014	0.013	-74.81185183	-75.02779987	-75.03119727
O	CV	4	3	8	6	84	0.222	0.212	-74.81732590	-75.05009728	-75.05420818
O	CV	5	3	8	6	145	2.125	2.071	-74.81878772	-75.05705314	-75.06140368
O	FC	2	3	8	6	18	0.002	0.002	-74.79228596	-74.91497714	-74.91587772
O	FC	3	3	8	6	43	0.013	0.012	-74.81185183	-74.97566730	-74.97880038
O	FC	4	3	8	6	84	0.204	0.198	-74.81732590	-74.99181195	-74.99560778
O	FC	5	3	8	6	145	2.025	1.99	-74.81878772	-74.99696897	-75.00099213
P	CV	2	4	15	5	27	0.004	0.003	-340.70924975	-340.94096681	-340.94337961
P	CV	3	4	15	5	59	0.051	0.042	-340.71644935	-341.10711594	-341.11360486
P	CV	4	4	15	5	109	0.591	0.536	-340.71882144	-341.18694401	-341.19477656
P	CV	5	4	15	5	181	4.603	4.222	-340.71916916	-341.22143701	-341.22967021
P	FC	2	4	15	5	27	0.002	0.002	-340.70924975	-340.79320545	-340.79438646
P	FC	3	4	15	5	59	0.033	0.032	-340.71644935	-340.81866817	-340.82265525
P	FC	4	4	15	5	109	0.459	0.451	-340.71882144	-340.82441826	-340.82905789
P	FC	5	4	15	5	181	3.785	3.741	-340.71916916	-340.82577534	-340.83057819
S	CV	2	3	16	6	27	0.004	0.003	-397.49725711	-397.75381722	-397.75638667
S	CV	3	3	16	6	59	0.055	0.046	-397.50955947	-397.94473562	-397.95209822
S	CV	4	3	16	6	109	0.644	0.582	-397.51274737	-398.03254786	-398.04152958
S	CV	5	3	16	6	181	5.109	4.652	-397.51321879	-398.06942699	-398.07888523
S	FC	2	3	16	6	27	0.002	0.002	-397.49725711	-397.60453364	-397.60596285
S	FC	3	3	16	6	59	0.033	0.032	-397.50955947	-397.65166417	-397.65663671
S	FC	4	3	16	6	109	0.508	0.496	-397.51274737	-397.66321977	-397.66914920
S	FC	5	3	16	6	181	4.164	4.099	-397.51321879	-397.66618226	-397.67236383
Si	CV	2	3	14	4	27	0.004	0.003	-288.85031171	-289.05703463	-289.05956570
Si	CV	3	3	14	4	59	0.053	0.046	-288.85657424	-289.21580311	-289.22115385
Si	CV	4	3	14	4	109	0.633	0.58	-288.85854384	-289.28993851	-289.29640864
Si	CV	5	3	14	4	181	4.955	4.608	-288.85884514	-289.32409204	-289.33091565

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SD(T), min	Time SD, min	HF	CCSD	CCSD(T)
Si	FC	2	3	14	4	27	0.002	0.002	-288.85031171	-288.91568750	-288.91677377
Si	FC	3	3	14	4	59	0.037	0.036	-288.85657424	-288.93145645	-288.93398966
Si	FC	4	3	14	4	109	0.519	0.512	-288.85854384	-288.93541975	-288.93829826
Si	FC	5	3	14	4	181	4.171	4.138	-288.85884514	-288.93624648	-288.93920499

Table S17. Raw data for SDT(Q)/nZ (n = D, T, Q) computations. System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons (N_{val_el}), number of basis functions (Basis size), time for SDT(Q) computation, (Time SDT(Q)), time for SDT computation (Time SDT), and energy components in Hartree (CCSDT, CCSDT(Q)) are provided.

System	CV	Cardinal	M	N_{el}	N_{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
alh	CV	2	1	14	4	32	0.384	0.327	-242.66217920	-242.66217499
alh	CV	3	1	14	4	73	10.421	5.292	-242.82709829	-242.82721781
alh	CV	4	1	14	4	139	220.109	53.958	-242.90153514	-242.90167104
alh	FC	2	1	14	4	32	0.018	0.015	-242.53058010	-242.53061025
alh	FC	3	1	14	4	73	0.65	0.461	-242.54714037	-242.54718924
alh	FC	4	1	14	4	139	10.626	5.43	-242.55114497	-242.55120093
bf	CV	2	1	14	10	36	0.682	0.552	-124.44969682	-124.45029410
bf	CV	3	1	14	10	86	22.314	10.721	-124.61102823	-124.61157377
bf	CV	4	1	14	10	168	629.389	153.507	-124.65391963	-124.65452338
bf	FC	2	1	14	10	36	0.261	0.208	-124.39038814	-124.39096091
bf	FC	3	1	14	10	86	9.255	4.549	-124.51128447	-124.51178960
bf	FC	4	1	14	10	168	234.94	56.477	-124.54228183	-124.54283936
bh	CV	2	1	6	4	23	0.022	0.018	-25.24466240	-25.24472349
bh	CV	3	1	6	4	57	0.622	0.397	-25.27621373	-25.27629053
bh	CV	4	1	6	4	114	11.338	4.608	-25.28491757	-25.28500056
bh	FC	2	1	6	4	23	0.01	0.009	-25.21673344	-25.21678592
bh	FC	3	1	6	4	57	0.305	0.228	-25.23222055	-25.23228755
bh	FC	4	1	6	4	114	5.268	3.092	-25.23580857	-25.23588044
bh3	CV	2	1	8	6	33	0.13	0.099	-26.53911619	-26.53915362
bh3	CV	3	1	8	6	85	5.224	2.292	-26.58480593	-26.58485240
bh3	CV	4	1	8	6	174	164.84	33.959	-26.59634236	-26.59639709
bh3	FC	2	1	8	6	33	0.064	0.048	-26.51057689	-26.51061114
bh3	FC	3	1	8	6	85	2.93	1.388	-26.53953745	-26.53958139
bh3	FC	4	1	8	6	174	87.911	20.814	-26.54582660	-26.54587832
cf	CV	2	2	15	11	36	1.296	1.045	-137.54769937	-137.54831640
cf	CV	3	2	15	11	86	59.976	25.721	-137.71682263	-137.71743332
cf	CV	4	2	15	11	168	1517.935	357.734	-137.76329970	-137.76398389
cf	FC	2	2	15	11	36	0.49	0.411	-137.48710218	-137.48769305
cf	FC	3	2	15	11	86	26.083	11.065	-137.61446717	-137.61503171

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
cf	FC	4	2	15	11	168	646.42	141.438	-137.64885510	-137.64948544
ch	CV	2	2	7	5	23	0.053	0.045	-38.41238313	-38.41245492
ch	CV	3	2	7	5	57	1.809	1.031	-38.45995091	-38.46004007
ch	CV	4	2	7	5	114	34.293	11.079	-38.47251288	-38.47261618
ch	FC	2	2	7	5	23	0.029	0.024	-38.38296575	-38.38302968
ch	FC	3	2	7	5	57	0.866	0.578	-38.41295889	-38.41303674
ch	FC	4	2	7	5	114	15.105	6.483	-38.42010653	-38.42019609
ch2-sing	CV	2	1	8	6	28	0.084	0.07	-39.05535217	-39.05551604
ch2-sing	CV	3	1	8	6	71	2.841	1.641	-39.11159461	-39.11180062
ch2-sing	CV	4	1	8	6	144	64.309	19.16	-39.12624246	-39.12647422
ch2-sing	FC	2	1	8	6	28	0.044	0.037	-39.02562706	-39.02578173
ch2-sing	FC	3	1	8	6	71	1.612	0.971	-39.06417644	-39.06436986
ch2-sing	FC	4	1	8	6	144	35.682	12.293	-39.07337446	-39.07359111
ch2-trip	CV	2	3	8	6	28	0.124	0.095	-39.07419265	-39.07426593
ch2-trip	CV	3	3	8	6	71	5.266	2.286	-39.12807200	-39.12815194
ch2-trip	CV	4	3	8	6	144	139.237	30.262	-39.14181375	-39.14190935
ch2-trip	FC	2	3	8	6	28	0.06	0.048	-39.04426391	-39.04433229
ch2-trip	FC	3	3	8	6	71	2.571	1.311	-39.08017367	-39.08024721
ch2-trip	FC	4	3	8	6	144	64.349	17.358	-39.08841616	-39.08850380
ch3	CV	2	2	9	7	33	0.298	0.206	-39.74914849	-39.74926326
ch3	CV	3	2	9	7	85	15.47	5.3	-39.81170553	-39.81182612
ch3	CV	4	2	9	7	174	501.427	81.655	-39.82737017	-39.82751231
ch3	FC	2	2	9	7	33	0.166	0.115	-39.71886464	-39.71897309
ch3	FC	3	2	9	7	85	8.58	3.048	-39.76340053	-39.76351476
ch3	FC	4	2	9	7	174	283.398	46.327	-39.77354085	-39.77367528
cn	CV	2	2	13	9	36	1.157	0.986	-92.55966804	-92.56176145
cn	CV	3	2	13	9	86	45.669	21.31	-92.62851711	-92.63042522
cn	CV	4	2	13	9	168	1079.502	252.522	-92.65578053	-92.65761646
cn	FC	2	2	13	9	36	0.39	0.335	-92.49933819	-92.50137615
cn	FC	3	2	13	9	86	17.411	7.632	-92.53030026	-92.53214250
cn	FC	4	2	13	9	168	423.894	92.819	-92.54613929	-92.54791118
co	CV	2	1	14	10	36	0.685	0.555	-113.12541643	-113.12651893
co	CV	3	1	14	10	86	21.362	10.042	-113.26454277	-113.26573761
co	CV	4	1	14	10	168	620.952	144.585	-113.30335776	-113.30464777

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
co	FC	2	1	14	10	36	0.263	0.209	-113.06489198	-113.06595928
co	FC	3	1	14	10	86	8.936	4.249	-113.16387727	-113.16502129
co	FC	4	1	14	10	168	232.761	56.784	-113.19091010	-113.19214233
f2	CV	2	1	18	14	36	0.678	0.465	-199.17650779	-199.17816035
f2	CV	3	1	18	14	86	29.785	11.047	-199.42051850	-199.42214153
f2	CV	4	1	18	14	168	728.09	131.401	-199.48856241	-199.49033942
f2	FC	2	1	18	14	36	0.397	0.283	-199.11460051	-199.11622734
f2	FC	3	1	18	14	86	14.853	5.538	-199.31036637	-199.31195269
f2	FC	4	1	18	14	168	335.119	59.663	-199.36511923	-199.36685104
h2o	CV	2	1	10	8	28	0.113	0.092	-76.27845597	-76.27892310
h2o	CV	3	1	10	8	71	4.296	2.251	-76.39016409	-76.39054543
h2o	CV	4	1	10	8	144	110.097	28.153	-76.42112532	-76.42156084
h2o	FC	2	1	10	8	28	0.065	0.053	-76.24748006	-76.24793683
h2o	FC	3	1	10	8	71	2.561	1.356	-76.33706430	-76.33742665
h2o	FC	4	1	10	8	144	62.097	16.814	-76.36177956	-76.36219122
h2s	CV	2	1	18	8	37	1.111	0.896	-399.02462515	-399.02489416
h2s	CV	3	1	18	8	87	43.639	17.789	-399.23769488	-399.23812512
h2s	CV	4	1	18	8	169	1241.699	213.642	-399.33242100	-399.33294622
h2s	FC	2	1	18	8	37	0.113	0.084	-398.87385805	-398.87409602
h2s	FC	3	1	18	8	87	4.768	2.125	-398.94160945	-398.94195986
h2s	FC	4	1	18	8	169	122.422	26.72	-398.95943587	-398.95986670
hcl	CV	2	1	18	8	32	0.434	0.345	-460.41569389	-460.41598198
hcl	CV	3	1	18	8	73	18.877	8.982	-460.64677245	-460.64717417
hcl	CV	4	1	18	8	139	457	112.947	-460.74641855	-460.74692766
hcl	FC	2	1	18	8	32	0.06	0.048	-460.26470626	-460.26496270
hcl	FC	3	1	18	8	73	2.217	1.146	-460.34385827	-460.34418115
hcl	FC	4	1	18	8	139	45.506	12.092	-460.36644969	-460.36686121
hf	CV	2	1	10	8	23	0.056	0.045	-100.26785989	-100.26825758
hf	CV	3	1	10	8	57	1.729	1.04	-100.40056590	-100.40083556
hf	CV	4	1	10	8	114	33.675	10.523	-100.43819603	-100.43850542
hf	FC	2	1	10	8	23	0.031	0.026	-100.23668288	-100.23707138
hf	FC	3	1	10	8	57	1.01	0.598	-100.34519971	-100.34544899
hf	FC	4	1	10	8	114	19.675	6.521	-100.37616385	-100.37644727
hs	CV	2	2	17	7	32	0.829	0.609	-398.38259190	-398.38277625

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
hs	CV	3	2	17	7	73	36.616	16.929	-398.58803998	-398.58834246
hs	CV	4	2	17	7	139	760.031	195.144	-398.68043207	-398.68081640
hs	FC	2	2	17	7	32	0.091	0.071	-398.23200091	-398.23215711
hs	FC	3	2	17	7	73	3.653	1.649	-398.29231639	-398.29253955
hs	FC	4	2	17	7	139	78.832	19.647	-398.30780462	-398.30809419
n2	CV	2	1	14	10	36	0.43	0.291	-109.34591435	-109.34761038
n2	CV	3	1	14	10	86	14.969	5.158	-109.48237926	-109.48424592
n2	CV	4	1	14	10	168	336.819	54.707	-109.51945144	-109.52143853
n2	FC	2	1	14	10	36	0.179	0.116	-109.28493267	-109.28659464
n2	FC	3	1	14	10	86	6.316	2.207	-109.38134745	-109.38317361
n2	FC	4	1	14	10	168	132.247	22.81	-109.40668062	-109.40862184
nh	CV	2	3	8	6	23	0.059	0.049	-55.12602008	-55.12613331
nh	CV	3	3	8	6	57	2.152	1.178	-55.19414702	-55.19425701
nh	CV	4	3	8	6	114	44.94	13.619	-55.21194834	-55.21208098
nh	FC	2	3	8	6	23	0.03	0.025	-55.09579361	-55.09590090
nh	FC	3	3	8	6	57	1.061	0.644	-55.14414348	-55.14424257
nh	FC	4	3	8	6	114	20.467	7.164	-55.15614442	-55.15626301
nh2	CV	2	2	9	7	28	0.186	0.145	-55.76784443	-55.76806126
nh2	CV	3	2	9	7	71	7.765	3.585	-55.84747658	-55.84768655
nh2	CV	4	2	9	7	144	192.698	45.639	-55.86853405	-55.86877898
nh2	FC	2	2	9	7	28	0.096	0.074	-55.73728348	-55.73749262
nh2	FC	3	2	9	7	71	4.328	2.021	-55.79709424	-55.79729235
nh2	FC	4	2	9	7	144	109.228	26.274	-55.81232382	-55.81255359
nh3	CV	2	1	10	8	33	0.365	0.308	-56.43766347	-56.43798980
nh3	CV	3	1	10	8	85	16.597	7.901	-56.52740157	-56.52771876
nh3	CV	4	1	10	8	174	681.104	144.905	-56.55108132	-56.55144637
nh3	FC	2	1	10	8	33	0.204	0.17	-56.40668728	-56.40700396
nh3	FC	3	1	10	8	85	9.845	4.843	-56.47649833	-56.47680284
nh3	FC	4	1	10	8	174	394.256	80.484	-56.49431277	-56.49466204
no	CV	2	2	15	11	36	1.701	1.343	-129.67037223	-129.67186106
no	CV	3	2	15	11	86	62.884	28.657	-129.82893043	-129.83053802
no	CV	4	2	15	11	168	1052.587	337.936	-129.87324780	-129.87498687
no	FC	2	2	15	11	36	0.69	0.531	-129.60925950	-129.61071298
no	FC	3	2	15	11	86	26.831	11.872	-129.72581941	-129.72737848

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
no	FC	4	2	15	11	168	416.437	135.255	-129.75807794	-129.75976114
o2	CV	2	3	16	12	36	1.061	0.65	-150.05967915	-150.06156285
o2	CV	3	3	16	12	86	46.425	14.2	-150.24461196	-150.24649965
o2	CV	4	3	16	12	168	995.307	149.32	-150.29592613	-150.29794867
o2	FC	2	3	16	12	36	0.481	0.279	-149.99844998	-150.00030549
o2	FC	3	3	16	12	86	21.862	5.992	-150.13919773	-150.14104982
o2	FC	4	3	16	12	168	468.424	64.022	-150.17808229	-150.18006253
oh	CV	2	2	9	7	23	0.076	0.062	-75.59621903	-75.59646528
oh	CV	3	2	9	7	57	3.056	1.626	-75.69553353	-75.69572956
oh	CV	4	2	9	7	114	62.447	18.949	-75.72286392	-75.72309656
oh	FC	2	2	9	7	23	0.042	0.034	-75.56559094	-75.56582996
oh	FC	3	2	9	7	57	1.659	0.893	-75.64283436	-75.64301504
oh	FC	4	2	9	7	114	34.381	10.261	-75.66394539	-75.66415807
sih	CV	2	2	15	5	32	0.894	0.71	-289.66609263	-289.66614854
sih	CV	3	2	15	5	73	28.466	13.647	-289.83620784	-289.83637403
sih	CV	4	2	15	5	139	536.153	133.023	-289.91365985	-289.91385431
sih	FC	2	2	15	5	32	0.052	0.043	-289.52344679	-289.52349316
sih	FC	3	2	15	5	73	1.806	1.077	-289.54906867	-289.54915035
sih	FC	4	2	15	5	139	32.258	11.434	-289.55557146	-289.55567047
Al	CV	2	2	13	3	27	0.133	0.101	-242.05431894	-242.05429204
Al	CV	3	2	13	3	59	4.564	1.591	-242.21219575	-242.21228558
Al	CV	4	2	13	3	109	79.86	15.348	-242.28502837	-242.28513103
Al	FC	2	2	13	3	27	0.005	0.005	-241.92233030	-241.92233030
Al	FC	3	2	13	3	59	0.093	0.093	-241.93206870	-241.93206870
Al	FC	4	2	13	3	109	1.122	1.122	-241.93451220	-241.93451220
B	CV	2	2	5	3	18	0.009	0.007	-24.61908952	-24.61910023
B	CV	3	2	5	3	43	0.168	0.091	-24.64320882	-24.64322199
B	CV	4	2	5	3	84	2.462	0.895	-24.65031511	-24.65032982
B	FC	2	2	5	3	18	0.003	0.003	-24.59131471	-24.59131471
B	FC	3	2	5	3	43	0.04	0.04	-24.59953105	-24.59953105
B	FC	4	2	5	3	84	0.507	0.507	-24.60155388	-24.60155388
C	CV	2	3	6	4	18	0.009	0.007	-37.79242862	-37.79246032
C	CV	3	3	6	4	43	0.149	0.086	-37.82979088	-37.82983798
C	CV	4	3	6	4	84	3.254	0.993	-37.83975172	-37.83980636

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
C	FC	2	3	6	4	18	0.004	0.004	-37.76325429	-37.76327789
C	FC	3	3	6	4	43	0.056	0.044	-37.78308318	-37.78311815
C	FC	4	3	6	4	84	0.842	0.561	-37.78764952	-37.78768993
Cl	CV	2	2	17	7	27	0.258	0.177	-459.75812946	-459.75830896
Cl	CV	3	2	17	7	59	9.379	3.673	-459.98005085	-459.98029229
Cl	CV	4	2	17	7	109	148.925	29.806	-460.07677230	-460.07710284
Cl	FC	2	2	17	7	27	0.028	0.019	-459.60741570	-459.60756776
Cl	FC	3	2	17	7	59	0.967	0.321	-459.67755374	-459.67772353
Cl	FC	4	2	17	7	109	16.542	3.025	-459.69721610	-459.69745729
F	CV	2	2	9	7	18	0.021	0.016	-99.56677194	-99.56689113
F	CV	3	2	9	7	43	0.623	0.255	-99.68247466	-99.68255830
F	CV	4	2	9	7	84	10.933	2.455	-99.71524067	-99.71534940
F	FC	2	2	9	7	18	0.015	0.013	-99.53591115	-99.53602508
F	FC	3	2	9	7	43	0.343	0.143	-99.62744934	-99.62751998
F	FC	4	2	9	7	84	6.317	1.449	-99.65356465	-99.65365643
N	CV	2	4	7	5	18	0.009	0.007	-54.51247717	-54.51251840
N	CV	3	4	7	5	43	0.182	0.098	-54.56770223	-54.56775256
N	CV	4	4	7	5	84	4.603	1.137	-54.58176421	-54.58182838
N	FC	2	4	7	5	18	0.005	0.004	-54.48252774	-54.48256403
N	FC	3	4	7	5	43	0.07	0.049	-54.51795050	-54.51799050
N	FC	4	4	7	5	84	1.12	0.61	-54.52622532	-54.52627658
O	CV	2	3	8	6	18	0.016	0.013	-74.94630565	-74.94638281
O	CV	3	3	8	6	43	0.442	0.187	-75.03147798	-75.03154318
O	CV	4	3	8	6	84	7.935	1.832	-75.05451402	-75.05460141
O	FC	2	3	8	6	18	0.009	0.008	-74.91598359	-74.91605614
O	FC	3	3	8	6	43	0.212	0.102	-74.97908071	-74.97913461
O	FC	4	3	8	6	84	3.696	1.083	-74.99591306	-74.99598569
P	CV	2	4	15	5	27	0.182	0.113	-340.94362699	-340.94374325
P	CV	3	4	15	5	59	6.62	2.382	-341.11424643	-341.11446410
P	CV	4	4	15	5	109	102.456	17.336	-341.19537992	-341.19564447
P	FC	2	4	15	5	27	0.01	0.008	-340.79469629	-340.79477917
P	FC	3	4	15	5	59	0.277	0.159	-340.82343125	-340.82355516
P	FC	4	4	15	5	109	3.541	1.453	-340.82979487	-340.82995159
S	CV	2	3	16	6	27	0.207	0.135	-397.75663994	-397.75677664

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDT(Q), min	Time SDT, min	CCSDT	CCSDT(Q)
S	CV	3	3	16	6	59	8.339	3.335	-397.95275636	-397.95296993
S	CV	4	3	16	6	109	125.73	25.021	-398.04221424	-398.04249886
S	FC	2	3	16	6	27	0.024	0.017	-397.60627836	-397.60638554
S	FC	3	3	16	6	59	0.622	0.256	-397.65741986	-397.65755247
S	FC	4	3	16	6	109	9.867	2.3	-397.66995788	-397.67014618
Si	CV	2	3	14	4	27	0.176	0.113	-289.05992823	-289.05998148
Si	CV	3	3	14	4	59	6.316	2.455	-289.22179366	-289.22195351
Si	CV	4	3	14	4	109	91.556	17.354	-289.29700945	-289.29719423
Si	FC	2	3	14	4	27	0.009	0.008	-288.91719698	-288.91723406
Si	FC	3	3	14	4	59	0.198	0.136	-288.93473855	-288.93479992
Si	FC	4	3	14	4	109	2.463	1.426	-288.93900979	-288.93908245

Table S18. Raw data for SDTQ(P)/nZ (n = D, T) computations. System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons (N_{val_el}), number of basis functions (Basis size), time for SDTQ(P) computation, (Time SDTQ(P)), time for SDTQ computation (Time SDTQ), and energy components in Hartree (CCSDTQ, CCSDTQ(P)) are provided.

System	CV	Cardinal	M	N_{el}	N_{val_el}	Basis size	Time SDTQ(P), min	Time SDTQ, min	CCSDTQ	CCSDTQ(P)
bh3	CV	2	1	8	6	33	2.724	1.868	-26.53916039	-26.53916021
bh3	CV	3	1	8	6	85	331.571	114.353	-26.58485855	-26.58485513
bh3	FC	2	1	8	6	33	0.69	0.537	-26.51061771	-26.51061753
bh3	FC	3	1	8	6	85	70.391	29.286	-26.53958787	-26.53958503
ch	CV	2	2	7	5	23	0.396	0.323	-38.41246858	-38.41247018
ch	CV	3	2	7	5	57	46.362	22.625	-38.46005388	-38.46005372
ch	FC	2	2	7	5	23	0.084	0.075	-38.38304293	-38.38304438
ch	FC	3	2	7	5	57	7.125	4.163	-38.41305032	-38.41305029
ch2-sing	CV	2	1	8	6	28	1.849	1.495	-39.05554464	-39.05554845
ch2-sing	CV	3	1	8	6	71	126.109	64.096	-39.11183122	-39.11182980
ch2-sing	FC	2	1	8	6	28	0.465	0.378	-39.02581020	-39.02581382
ch2-sing	FC	3	1	8	6	71	31.17	17.028	-39.06440048	-39.06439948
ch2-trip	CV	2	3	8	6	28	2.127	1.457	-39.07427543	-39.07427742
ch2-trip	CV	3	3	8	6	71	213.494	70.729	-39.12815806	-39.12815789
ch2-trip	FC	2	3	8	6	28	0.517	0.375	-39.04434158	-39.04434341
ch2-trip	FC	3	3	8	6	71	40.09	15.37	-39.08025338	-39.08025325
ch3	CV	2	2	9	7	33	5.337	3.471	-39.74927060	-39.74927471
ch3	CV	3	2	9	7	85	1433.425	356.86	-39.81183262	-39.81183100
ch3	FC	2	2	9	7	33	1.801	1.16	-39.71898035	-39.71898423
ch3	FC	3	2	9	7	85	414.639	98.021	-39.76352172	-39.76352029
h2o	CV	2	1	10	8	28	3.26	2.407	-76.27889315	-76.27890913
h2o	CV	3	1	10	8	71	383.068	127.991	-76.39050973	-76.39052393
h2o	FC	2	1	10	8	28	1.457	1.066	-76.24790773	-76.24792311
h2o	FC	3	1	10	8	71	128.345	49.16	-76.33739230	-76.33740544
hf	CV	2	1	10	8	23	0.927	0.7	-100.26823280	-100.26824376
hf	CV	3	1	10	8	57	101.801	44.572	-100.40080497	-100.40081169
hf	FC	2	1	10	8	23	0.484	0.377	-100.23704749	-100.23705803
hf	FC	3	1	10	8	57	36.824	17.405	-100.34541945	-100.34542533
nh	CV	2	3	8	6	23	0.769	0.582	-55.12614754	-55.12615004

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDTQ(P), min	Time SDTQ, min	CCSDTQ	CCSDTQ(P)
nh	CV	3	3	8	6	57	56.71	26.124	-55.19426187	-55.19426346
nh	FC	2	3	8	6	23	0.193	0.155	-55.09591516	-55.09591745
nh	FC	3	3	8	6	57	12.199	6.32	-55.14424753	-55.14424885
nh2	CV	2	2	9	7	28	2.643	1.911	-55.76806726	-55.76807528
nh2	CV	3	2	9	7	71	528.478	174.939	-55.84768638	-55.84769089
nh2	FC	2	2	9	7	28	0.871	0.618	-55.73749879	-55.73750644
nh2	FC	3	2	9	7	71	164.695	55.622	-55.79729269	-55.79729683
oh	CV	2	2	9	7	23	0.847	0.663	-75.59647120	-75.59647719
oh	CV	3	2	9	7	57	154.119	63.842	-75.69572036	-75.69572539
oh	FC	2	2	9	7	23	0.332	0.259	-75.56583636	-75.56584201
oh	FC	3	2	9	7	57	49.694	20.349	-75.64300633	-75.64301079
Al	CV	2	2	13	3	27	4.33	2.097	-242.05429515	-242.05429325
Al	CV	3	2	13	3	59	525.31	123.936	-242.21228078	-242.21227879
Al	FC	2	2	13	3	27	0.005	0.005	-241.92233030	-241.92233030
Al	FC	3	2	13	3	59	0.094	0.094	-241.93206870	-241.93206870
B	CV	2	2	5	3	18	0.022	0.019	-24.61910083	-24.61910090
B	CV	3	2	5	3	43	1.08	0.493	-24.64322237	-24.64322241
B	FC	2	2	5	3	18	0.003	0.003	-24.59131471	-24.59131471
B	FC	3	2	5	3	43	0.038	0.038	-24.59953105	-24.59953105
C	CV	2	3	6	4	18	0.035	0.029	-37.79246871	-37.79246885
C	CV	3	3	6	4	43	1.799	0.819	-37.82984526	-37.82984540
C	FC	2	3	6	4	18	0.006	0.006	-37.76328615	-37.76328615
C	FC	3	3	6	4	43	0.111	0.111	-37.78312550	-37.78312550
Cl	CV	2	2	17	7	27	8.82	4.438	-459.75831804	-459.75832422
Cl	CV	3	2	17	7	59	1425.042	379.213	-459.98029337	-459.98029606
Cl	FC	2	2	17	7	27	0.228	0.149	-459.60758420	-459.60758889
Cl	FC	3	2	17	7	59	32.208	7.827	-459.67773175	-459.67773377
F	CV	2	2	9	7	18	0.151	0.102	-99.56689266	-99.56689790
F	CV	3	2	9	7	43	23.984	7.728	-99.68255289	-99.68255303
F	FC	2	2	9	7	18	0.076	0.058	-99.53602701	-99.53603209
F	FC	3	2	9	7	43	7.947	2.395	-99.62751477	-99.62751462
N	CV	2	4	7	5	18	0.048	0.037	-54.51252755	-54.51252802
N	CV	3	4	7	5	43	3.335	1.397	-54.56775555	-54.56775583
N	FC	2	4	7	5	18	0.012	0.01	-54.48257329	-54.48257367

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDTQ(P), min	Time SDTQ, min	CCSDTQ	CCSDTQ(P)
N	FC	3	4	7	5	43	0.415	0.224	-54.51799349	-54.51799359
O	CV	2	3	8	6	18	0.1	0.074	-74.94639101	-74.94639311
O	CV	3	3	8	6	43	8.518	3.233	-75.03154270	-75.03154310
O	FC	2	3	8	6	18	0.035	0.029	-74.91606461	-74.91606657
O	FC	3	3	8	6	43	1.949	0.848	-74.97913418	-74.97913435
P	CV	2	4	15	5	27	3.923	2.365	-340.94376384	-340.94376595
P	CV	3	4	15	5	59	569.292	158.274	-341.11447361	-341.11447646
P	FC	2	4	15	5	27	0.026	0.021	-340.79480621	-340.79480689
P	FC	3	4	15	5	59	1.465	0.664	-340.82357567	-340.82357684
S	CV	2	3	16	6	27	5.167	3.315	-397.75679175	-397.75679599
S	CV	3	3	16	6	59	786.623	262.657	-397.95297474	-397.95297673
S	FC	2	3	16	6	27	0.096	0.069	-397.60640692	-397.60640969
S	FC	3	3	16	6	59	7.423	2.564	-397.65756535	-397.65756651
Si	CV	2	3	14	4	27	3.874	2.455	-289.05999414	-289.05999474
Si	CV	3	3	14	4	59	485.817	144.855	-289.22195921	-289.22195973
Si	FC	2	3	14	4	27	0.012	0.012	-288.91724952	-288.91724952
Si	FC	3	3	14	4	59	0.309	0.309	-288.93481545	-288.93481545

Table S19. Raw data for SDTQP/nZ (n = D, T) computations. System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons ($N_{\text{val_el}}$), number of basis functions (Basis size), time for SDTQP computation, (Time SDTQP), and energy in Hartree (CCSDTQP) are provided.

System	CV	Cardinal	M	N_{el}	$N_{\text{val_el}}$	Basis size	Time SDTQP, min	CCSDTQP
bh3	CV	2	1	8	6	33	18.589	-26.53916083
bh3	CV	3	1	8	6	85	5714.978	-26.58485703
bh3	FC	2	1	8	6	33	2.512	-26.51061806
bh3	FC	3	1	8	6	85	811.759	-26.53958656
ch2-sing	CV	2	1	8	6	28	9.359	-39.05555089
ch2-sing	CV	3	1	8	6	71	2605.35	-39.11183520
ch2-sing	FC	2	1	8	6	28	1.617	-39.02581597
ch2-sing	FC	3	1	8	6	71	198.975	-39.06440400
h2o	CV	2	1	10	8	28	21.137	-76.27890987
h2o	CV	3	1	10	8	71	8699.435	-76.39052858
h2o	FC	2	1	10	8	28	6.642	-76.24792386
h2o	FC	3	1	10	8	71	2172.404	-76.33740995
hf	CV	2	1	10	8	23	5.685	-100.26824396
hf	CV	3	1	10	8	57	3097.99	-100.40081521
hf	FC	2	1	10	8	23	1.643	-100.23705822
hf	FC	3	1	10	8	57	398.438	-100.34542881
B	CV	2	2	5	3	18	0.03	-24.61910091
B	CV	3	2	5	3	43	1.641	-24.64322243
B	FC	2	2	5	3	18	0.003	-24.59131471
B	FC	3	2	5	3	43	0.039	-24.59953105
C	CV	2	3	6	4	18	0.065	-37.79246889
C	CV	3	3	6	4	43	4.676	-37.82984552
C	FC	2	3	6	4	18	0.007	-37.76328615
C	FC	3	3	6	4	43	0.125	-37.78312550
F	CV	2	2	9	7	18	0.488	-99.56689834
F	CV	3	2	9	7	43	117.583	-99.68255396
F	FC	2	2	9	7	18	0.161	-99.53603252
F	FC	3	2	9	7	43	24.962	-99.62751551
O	CV	2	3	8	6	18	0.289	-74.94639362

System	CV	Cardinal	M	N_{el}	N_{val_el}	Basis size	Time SDTQP, min	CCSDTQP
O	CV	3	3	8	6	43	53.772	-75.03154369
O	FC	2	3	8	6	18	0.075	-74.91606707
O	FC	3	3	8	6	43	7.102	-74.97913487

Table S20. Raw data for SDT(Q)/anZ (n = D, T, Q) computations. System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons (N_{val_el}), number of basis functions (Basis size), time for SDT(Q) computation, (Time SDT(Q)), time for SDT computation (Time SDT), and energy components in Hartree (HF, CCSD, CCSD(T), CCSDT, CCSDT(Q)) are provided.

System	CV	Cardinal	M	N_{el}	N_{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
alh	CV	2	1	14	4	45	1.503	1.109	-242.45548109	-242.66273330	-242.66579276	-242.66616110	-242.66616459
alh	CV	3	1	14	4	98	39.457	14.962	-242.46268591	-242.82297802	-242.82783768	-242.82819533	-242.82831966
alh	CV	4	1	14	4	180	896.143	183.197	-242.46426772	-242.89567388	-242.90153830	-242.90186246	-242.90199972
alh	FC	2	1	14	4	45	0.083	0.068	-242.45548109	-242.53232752	-242.53348638	-242.53387284	-242.53390959
alh	FC	3	1	14	4	98	2.356	1.514	-242.46268591	-242.54615282	-242.54766503	-242.54804765	-242.54810025
alh	FC	4	1	14	4	180	38.853	16.526	-242.46426772	-242.54943023	-242.55104711	-242.55139833	-242.55145555
bh	CV	2	1	6	4	36	0.113	0.088	-25.12657759	-25.24555456	-25.24741407	-25.24786849	-25.24793723
bh	CV	3	1	6	4	82	2.845	1.575	-25.13038518	-25.27383952	-25.27652113	-25.27699235	-25.27707277
bh	CV	4	1	6	4	155	49.136	15.373	-25.13140703	-25.28187606	-25.28471575	-25.28515742	-25.28524174
bh	FC	2	1	6	4	36	0.054	0.044	-25.12657759	-25.21779143	-25.21936076	-25.21980269	-25.21986210
bh	FC	3	1	6	4	82	1.366	0.936	-25.13038518	-25.23039578	-25.23255509	-25.23298882	-25.23305919
bh	FC	4	1	6	4	155	21.855	10.716	-25.13140703	-25.23337958	-25.23564339	-25.23604564	-25.23611881
ch	CV	2	2	7	5	36	0.221	0.176	-38.27558801	-38.41668058	-38.41930847	-38.41992348	-38.42001101
ch	CV	3	2	7	5	82	5.359	3.053	-38.28229881	-38.45749747	-38.46151677	-38.46221035	-38.46231017
ch	CV	4	2	7	5	155	155.476	38.275	-38.28401537	-38.46834147	-38.47262519	-38.47327890	-38.47338689
ch	FC	2	2	7	5	36	0.109	0.09	-38.27558801	-38.38734668	-38.38975547	-38.39036295	-38.39044027
ch	FC	3	2	7	5	82	2.704	1.768	-38.28229881	-38.41093891	-38.41454531	-38.41521084	-38.41529775
ch	FC	4	2	7	5	155	67.296	22.809	-38.28401537	-38.41643006	-38.42025208	-38.42087428	-38.42096804
ch2-sing	CV	2	1	8	6	45	0.518	0.385	-38.88464723	-39.05988815	-39.06380956	-39.06459827	-39.06479204
ch2-sing	CV	3	1	8	6	105	15.206	6.57	-38.89354886	-39.10800337	-39.11367936	-39.11454655	-39.11477029
ch2-sing	CV	4	1	8	6	201	382.731	84.074	-38.89546774	-39.12040422	-39.12641846	-39.12724848	-39.12748784
ch2-sing	FC	2	1	8	6	45	0.277	0.207	-38.88464723	-39.03025287	-39.03392788	-39.03469423	-39.03487679
ch2-sing	FC	3	1	8	6	105	8.68	4.034	-38.89354886	-39.06108225	-39.06630403	-39.06710954	-39.06731930
ch2-sing	FC	4	1	8	6	201	204.95	47.414	-38.89546774	-39.06811105	-39.07361865	-39.07437948	-39.07460331
ch2-trip	CV	2	3	8	6	45	0.566	0.4	-38.92849911	-39.07801388	-39.08054598	-39.08100732	-39.08109032
ch2-trip	CV	3	3	8	6	105	19.12	7.809	-38.93827206	-39.12559389	-39.12960314	-39.13011532	-39.13020580
ch2-trip	CV	4	3	8	6	201	503.273	110.58	-38.94034843	-39.13770144	-39.14200991	-39.14248347	-39.14258319
ch2-trip	FC	2	3	8	6	45	0.28	0.205	-38.92849911	-39.04804992	-39.05044169	-39.05090138	-39.05097806
ch2-trip	FC	3	3	8	6	105	9.383	4.33	-38.93827206	-39.07798149	-39.08169896	-39.08219852	-39.08228149

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
ch2-trip	FC	4	3	8	6	201	247.431	61.185	-38.94034843	-39.08465434	-39.08862682	-39.08908548	-39.08917693
h2o	CV	2	1	10	8	45	0.765	0.545	-76.04155800	-76.30508411	-76.31093082	-76.31109633	-76.31159572
h2o	CV	3	1	10	8	105	24.687	9.632	-76.06068649	-76.39050101	-76.39983174	-76.39986483	-76.40029028
h2o	CV	4	1	10	8	201	641.382	123.166	-76.06596896	-76.41480779	-76.42476010	-76.42473376	-76.42519480
h2o	FC	2	1	10	8	45	0.441	0.308	-76.04155800	-76.27412080	-76.27979992	-76.27996979	-76.28045403
h2o	FC	3	1	10	8	105	13.9	5.416	-76.06068649	-76.33777859	-76.34673569	-76.34676509	-76.34716651
h2o	FC	4	1	10	8	201	376.369	71.899	-76.06596896	-76.35590785	-76.36543115	-76.36539649	-76.36583156
hcl	CV	2	1	18	8	45	2.394	1.759	-460.09476058	-460.42831169	-460.43416628	-460.43446913	-460.43485721
hcl	CV	3	1	18	8	98	76.869	28.419	-460.10884558	-460.64090073	-460.65244788	-460.65285092	-460.65331668
hcl	CV	4	1	18	8	180	1801.263	349.606	-460.11212603	-460.73491743	-460.74807731	-460.74843444	-460.74896930
hcl	FC	2	1	18	8	45	0.277	0.194	-460.09476058	-460.27777380	-460.28233558	-460.28272600	-460.28307238
hcl	FC	3	1	18	8	98	8.575	3.566	-460.10884558	-460.34000631	-460.34909291	-460.34964278	-460.35001680
hcl	FC	4	1	18	8	180	180.33	37.466	-460.11212603	-460.35779571	-460.36788404	-460.36838027	-460.36881410
hf	CV	2	1	10	8	36	0.306	0.235	-100.03353372	-100.29848065	-100.30325500	-100.30338454	-100.30374110
hf	CV	3	1	10	8	82	7.668	3.657	-100.06113323	-100.40317292	-100.41140739	-100.41138968	-100.41167700
hf	CV	4	1	10	8	155	160.224	40.183	-100.06857916	-100.43339796	-100.44225124	-100.44217862	-100.44250529
hf	FC	2	1	10	8	36	0.173	0.131	-100.03353372	-100.26727864	-100.27190975	-100.27204500	-100.27238810
hf	FC	3	1	10	8	82	4.668	2.206	-100.06113323	-100.34813366	-100.35603227	-100.35602474	-100.35628632
hf	FC	4	1	10	8	155	92.788	22.396	-100.06857916	-100.37175751	-100.38022072	-100.38015659	-100.38045515
hs	CV	2	2	17	7	45	3.318	2.607	-398.09441097	-398.39109235	-398.39617609	-398.39671186	-398.39696714
hs	CV	3	2	17	7	98	95.407	42.979	-398.10734459	-398.58213699	-398.59164030	-398.59238782	-398.59273593
hs	CV	4	2	17	7	180	2892.256	643.921	-398.11029898	-398.67021115	-398.68112550	-398.68182695	-398.68222900
hs	FC	2	2	17	7	45	0.309	0.227	-398.09441097	-398.24111191	-398.24485236	-398.24547101	-398.24568844
hs	FC	3	2	17	7	98	9.207	4.264	-398.10734459	-398.28859321	-398.29558140	-398.29645589	-398.29671481
hs	FC	4	2	17	7	180	300.002	57.362	-398.11029898	-398.30056852	-398.30831279	-398.30913383	-398.30943852
nh	CV	2	3	8	6	36	0.272	0.216	-54.97218218	-55.13719904	-55.13999073	-55.14042035	-55.14054961
nh	CV	3	3	8	6	82	6.534	3.551	-54.98270341	-55.19320968	-55.19790517	-55.19839909	-55.19852795
nh	CV	4	3	8	6	155	126.354	39.409	-54.98559399	-55.20793548	-55.21299750	-55.21344963	-55.21359171
nh	FC	2	3	8	6	36	0.136	0.11	-54.97218218	-55.10696499	-55.10961180	-55.11004192	-55.11016214
nh	FC	3	3	8	6	82	3.421	2.04	-54.98270341	-55.14352703	-55.14790847	-55.14839610	-55.14851113
nh	FC	4	3	8	6	155	62.711	21.93	-54.98559399	-55.15250543	-55.15720704	-55.15765082	-55.15777777
nh2	CV	2	2	9	7	45	0.913	0.686	-55.57536280	-55.78223614	-55.78658319	-55.78702260	-55.78727328
nh2	CV	3	2	9	7	105	27.308	12.066	-55.58821629	-55.84622498	-55.85299550	-55.85343049	-55.85367149

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
nh2	CV	4	2	9	7	201	1111.904	204.276	-55.59139345	-55.86310138	-55.87032445	-55.87070844	-55.87096908
nh2	FC	2	2	9	7	45	0.503	0.373	-55.57536280	-55.75167762	-55.75585724	-55.75629677	-55.75653626
nh2	FC	3	2	9	7	105	15.71	6.99	-55.58821629	-55.79620765	-55.80262057	-55.80304157	-55.80326730
nh2	FC	4	2	9	7	201	624.884	116.119	-55.59139345	-55.80732192	-55.81413648	-55.81450243	-55.81474652
oh	CV	2	2	9	7	36	0.378	0.303	-75.40377876	-75.61690549	-75.62074107	-75.62106853	-75.62132204
oh	CV	3	2	9	7	82	9.022	4.997	-75.42176498	-75.69632995	-75.70282216	-75.70314567	-75.70337016
oh	CV	4	2	9	7	155	288.736	67.362	-75.42666849	-75.71833565	-75.72532780	-75.72560696	-75.72585689
oh	FC	2	2	9	7	36	0.206	0.161	-75.40377876	-75.58627307	-75.58995746	-75.59028736	-75.59052968
oh	FC	3	2	9	7	82	5.298	2.914	-75.42176498	-75.64397659	-75.65013050	-75.65045324	-75.65065780
oh	FC	4	2	9	7	155	162.604	38.005	-75.42666849	-75.65981935	-75.66642201	-75.66669795	-75.66692612
sih	CV	2	2	15	5	45	2.535	1.977	-289.43190008	-289.66743489	-289.67117241	-289.67178300	-289.67185820
sih	CV	3	2	15	5	98	68.671	30.956	-289.44032345	-289.83107605	-289.83724928	-289.83799792	-289.83817689
sih	CV	4	2	15	5	180	2113.153	460.531	-289.44247034	-289.90628909	-289.91350852	-289.91419969	-289.91439817
sih	FC	2	2	15	5	45	0.169	0.135	-289.43190008	-289.52580878	-289.52793775	-289.52860897	-289.52866953
sih	FC	3	2	15	5	98	4.6	2.746	-289.44032345	-289.54661828	-289.54985321	-289.55067862	-289.55076931
sih	FC	4	2	15	5	180	122.957	34.333	-289.44247034	-289.55177038	-289.55527085	-289.55603481	-289.55613716
Al	CV	2	2	13	3	36	0.442	0.3	-241.87427740	-242.05308553	-242.05566446	-242.05604412	-242.05602075
Al	CV	3	2	13	3	75	14.184	3.992	-241.87924597	-242.20777522	-242.21216352	-242.21258500	-242.21267706
Al	CV	4	2	13	3	134	197.118	30.6	-241.88050267	-242.27937609	-242.28474957	-242.28512684	-242.28522971
Al	FC	2	2	13	3	36	0.011	0.011	-241.87427740	-241.92254684	-241.92336853	-241.92378883	-241.92378883
Al	FC	3	2	13	3	75	0.231	0.231	-241.87924597	-241.93067732	-241.93188003	-241.93237202	-241.93237202
Al	FC	4	2	13	3	134	2.44	2.44	-241.88050267	-241.93282379	-241.93412574	-241.93457728	-241.93457728
B	CV	2	2	5	3	27	0.033	0.024	-24.53058146	-24.61925669	-24.62042882	-24.62083353	-24.62084563
B	CV	3	2	5	3	59	0.594	0.28	-24.53221572	-24.64124940	-24.64309205	-24.64354614	-24.64355990
B	CV	4	2	5	3	109	7.317	2.435	-24.53300052	-24.64803008	-24.64999865	-24.65042118	-24.65043602
B	FC	2	2	5	3	27	0.007	0.007	-24.53058146	-24.59166843	-24.59260484	-24.59300528	-24.59300528
B	FC	3	2	5	3	59	0.123	0.123	-24.53221572	-24.59802583	-24.59943095	-24.59986877	-24.59986877
B	FC	4	2	5	3	109	1.229	1.229	-24.53300052	-24.59976827	-24.60125406	-24.60166054	-24.60166054
C	CV	2	3	6	4	27	0.03	0.023	-37.68779748	-37.79512520	-37.79661340	-37.79700823	-37.79704938
C	CV	3	3	6	4	59	0.601	0.309	-37.69187228	-37.82769652	-37.83030273	-37.83080966	-37.83086191
C	CV	4	3	6	4	109	10.229	2.877	-37.69337496	-37.83678361	-37.83960660	-37.84007295	-37.84012945
C	FC	2	3	6	4	27	0.013	0.011	-37.68779748	-37.76604417	-37.76735810	-37.76775081	-37.76778166
C	FC	3	3	6	4	59	0.22	0.168	-37.69187228	-37.78133785	-37.78360750	-37.78410502	-37.78414388

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
C	FC	4	3	6	4	109	2.805	1.699	-37.69337496	-37.78507276	-37.78751701	-37.78797281	-37.78801478
Cl	CV	2	2	17	7	36	0.816	0.576	-459.47321127	-459.76837596	-459.77231850	-459.77266836	-459.77292057
Cl	CV	3	2	17	7	75	26.914	8.949	-459.48623678	-459.97498958	-459.98403215	-459.98463268	-459.98492399
Cl	CV	4	2	17	7	134	372.251	63.766	-459.48932510	-460.06710139	-460.07765656	-460.07823249	-460.07858218
Cl	FC	2	2	17	7	36	0.078	0.052	-459.47321127	-459.61810946	-459.62086545	-459.62128775	-459.62150407
Cl	FC	3	2	17	7	75	2.781	0.829	-459.48623678	-459.67447736	-459.68117842	-459.68191398	-459.68212137
Cl	FC	4	2	17	7	134	43.318	7.107	-459.48932510	-459.69029045	-459.69790115	-459.69860791	-459.69886512
F	CV	2	2	9	7	27	0.076	0.056	-99.38113528	-99.58656768	-99.58927299	-99.58946436	-99.58954758
F	CV	3	2	9	7	59	1.588	0.742	-99.40694448	-99.68471552	-99.68966804	-99.68986741	-99.68996411
F	CV	4	2	9	7	109	20.4	5.543	-99.41411220	-99.71226537	-99.71767032	-99.71783977	-99.71795947
F	FC	2	2	9	7	27	0.042	0.032	-99.38113528	-99.55566983	-99.55825840	-99.55845162	-99.55852701
F	FC	3	2	9	7	59	0.896	0.415	-99.40694448	-99.62996581	-99.63464201	-99.63484622	-99.63492615
F	FC	4	2	9	7	109	12.049	3.359	-99.41411220	-99.65091865	-99.65599963	-99.65617314	-99.65627449
N	CV	2	4	7	5	27	0.033	0.025	-54.39326499	-54.51936825	-54.52083635	-54.52108144	-54.52113024
N	CV	3	4	7	5	59	0.684	0.327	-54.40121154	-54.56650328	-54.56945176	-54.56981437	-54.56987525
N	CV	4	4	7	5	109	8.795	2.658	-54.40383912	-54.57885619	-54.58210609	-54.58243160	-54.58250025
N	FC	2	4	7	5	27	0.015	0.012	-54.39326499	-54.48941856	-54.49077590	-54.49102116	-54.49106260
N	FC	3	4	7	5	59	0.253	0.16	-54.40121154	-54.51700331	-54.51970513	-54.52006848	-54.52011701
N	FC	4	4	7	5	109	3.188	1.608	-54.40383912	-54.52360772	-54.52657074	-54.52689644	-54.52695161
O	CV	2	3	8	6	27	0.078	0.052	-74.79669729	-74.95981945	-74.96191746	-74.96218153	-74.96225420
O	CV	3	3	8	6	59	1.82	0.695	-74.81306194	-75.03212611	-75.03604535	-75.03638860	-75.03646986
O	CV	4	3	8	6	109	24.768	5.123	-74.81765587	-75.05157727	-75.05587043	-75.05618387	-75.05628007
O	FC	2	3	8	6	27	0.039	0.028	-74.79669729	-74.92948767	-74.93146673	-74.93173120	-74.93179660
O	FC	3	3	8	6	59	0.872	0.381	-74.81306194	-74.98001204	-74.98365889	-74.98400274	-74.98406948
O	FC	4	3	8	6	109	11.729	3.099	-74.81765587	-74.99330259	-74.99727854	-74.99759165	-74.99767199
P	CV	2	4	15	5	36	0.498	0.34	-340.71016765	-340.94616649	-340.94918620	-340.94954381	-340.94969647
P	CV	3	4	15	5	75	10.874	4.202	-340.71661072	-341.10817891	-341.11487930	-341.11556854	-341.11580594
P	CV	4	4	15	5	134	155.353	31.887	-340.71884321	-341.18725878	-341.19515753	-341.19575842	-341.19602932
P	FC	2	4	15	5	36	0.023	0.019	-340.71016765	-340.79804231	-340.79976016	-340.80018854	-340.80029863
P	FC	3	4	15	5	75	0.534	0.323	-340.71661072	-340.81959695	-340.82378954	-340.82461810	-340.82475561
P	FC	4	4	15	5	134	6.704	2.931	-340.71884321	-340.82468726	-340.82939359	-340.83012866	-340.83029077
S	CV	2	3	16	6	36	0.957	0.61	-397.49920841	-397.76353323	-397.76707106	-397.76749471	-397.76768745
S	CV	3	3	16	6	75	23.368	7.633	-397.51015949	-397.94723688	-397.95498440	-397.95570600	-397.95595351

System	CV	Cardinal	M	N _{el}	N _{val,el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
S	CV	4	3	16	6	134	317.555	57.716	-397.51285896	-398.03332728	-398.04242292	-398.04310858	-398.04340549
S	FC	2	3	16	6	36	0.076	0.05	-397.49920841	-397.61380121	-397.61609563	-397.61659337	-397.61674735
S	FC	3	3	16	6	75	1.858	0.682	-397.51015949	-397.65402603	-397.65936318	-397.66021417	-397.66037140
S	FC	4	3	16	6	134	25.374	5.553	-397.51285896	-397.66395720	-397.66999715	-397.67080773	-397.67100610
Si	CV	2	3	14	4	36	0.684	0.41	-288.85117655	-289.06024460	-289.06311754	-289.06356653	-289.06363535
Si	CV	3	3	14	4	75	16.826	5.009	-288.85676433	-289.21649486	-289.22195337	-289.22262846	-289.22279776
Si	CV	4	3	14	4	134	227.017	35.887	-288.85855950	-289.29012855	-289.29663082	-289.29722769	-289.29741479
Si	FC	2	3	14	4	36	0.025	0.021	-288.85117655	-288.91859516	-288.91996922	-288.92048381	-288.92052965
Si	FC	3	3	14	4	75	0.549	0.36	-288.85676433	-288.93203158	-288.93466753	-288.93545584	-288.93552217
Si	FC	4	3	14	4	134	6.141	3.3	-288.85855950	-288.93556412	-288.93847507	-288.93918284	-288.93925732

Table S21. Raw data for SDT(Q)/nZ (n = D, T, Q) computations. The geometries were optimized using SD(T)/nZ method with the basis set and frozen core approximation type corresponding to the given energy evaluation (FC-SD(T) for the FC single-point computation and CV-SD(T) for the CV one). System name (System), core electrons treatment (CV), basis set cardinal number (Cardinal), multiplicity (M), total number of electrons (N_{el}), number of valence electrons ($N_{val_{el}}$), number of basis functions (Basis size), time for SDT(Q) computation, (Time SDT(Q)), time for SDT computation (Time SDT), and energy components in Hartree (HF, CCSD, CCSD(T), CCSDT, CCSDT(Q)) are provided.

System	CV	Cardinal	M	N_{el}	$N_{val_{el}}$	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
alh	CV	2	1	14	4	32	0.528	0.408	-242.45506481	-242.65895817	-242.66184896	-242.66218621	-242.66218217
alh	CV	3	1	14	4	73	16.506	6.948	-242.46258338	-242.82196897	-242.82675183	-242.82710025	-242.82721962
alh	CV	4	1	14	4	139	337.848	63.11	-242.46424330	-242.89537597	-242.90121196	-242.90153948	-242.90167517
alh	FC	2	1	14	4	32	0.02	0.017	-242.45506621	-242.52920323	-242.53022997	-242.53058416	-242.53061436
alh	FC	3	1	14	4	73	0.893	0.584	-242.46258117	-242.54532245	-242.54676770	-242.54714035	-242.54718922
alh	FC	4	1	14	4	139	15.069	6.367	-242.46423992	-242.54919731	-242.55078984	-242.55114493	-242.55120087
bf	CV	2	1	14	10	36	0.918	0.677	-124.10759579	-124.44277369	-124.44986908	-124.45023790	-124.45085668
bf	CV	3	1	14	10	86	36.42	14.54	-124.15698939	-124.59851553	-124.61080397	-124.61103144	-124.61157541
bf	CV	4	1	14	10	168	978.41	172.641	-124.16615481	-124.64022575	-124.65378564	-124.65393622	-124.65453641
bf	FC	2	1	14	10	36	0.35	0.253	-124.10755118	-124.38388800	-124.39062828	-124.39098176	-124.39157653
bf	FC	3	1	14	10	86	14.769	5.583	-124.15686037	-124.49958036	-124.51109876	-124.51128606	-124.51179208
bf	FC	4	1	14	10	168	394.273	66.505	-124.16600393	-124.52949036	-124.54217483	-124.54228197	-124.54283916
bh	CV	2	1	6	4	23	0.028	0.022	-25.12539651	-25.24268233	-25.24439162	-25.24481577	-25.24487661
bh	CV	3	1	6	4	57	0.922	0.496	-25.13011366	-25.27312399	-25.27575035	-25.27621390	-25.27629068
bh	CV	4	1	6	4	114	18.314	5.543	-25.13135590	-25.28165787	-25.28447517	-25.28491982	-25.28500274
bh	FC	2	1	6	4	23	0.013	0.011	-25.12538601	-25.21505741	-25.21648534	-25.21689783	-25.21695004
bh	FC	3	1	6	4	57	0.431	0.3	-25.13008909	-25.22969046	-25.23179598	-25.23222201	-25.23228906
bh	FC	4	1	6	4	114	7.122	3.651	-25.13132917	-25.23315977	-25.23540314	-25.23580870	-25.23588059
bh3	CV	2	1	8	6	33	0.184	0.131	-26.39127217	-26.53733477	-26.53911323	-26.53947668	-26.53951489
bh3	CV	3	1	8	6	85	16.586	5.682	-26.40044593	-26.58147718	-26.58437868	-26.58480678	-26.58485321
bh3	CV	4	1	8	6	174	757.073	90.93	-26.40217395	-26.59279459	-26.59594302	-26.59634771	-26.59640233
bh3	FC	2	1	8	6	33	0.164	0.128	-26.39125711	-26.50897020	-26.51060578	-26.51096303	-26.51099809
bh3	FC	3	1	8	6	85	8.516	3.3	-26.40043137	-26.53652599	-26.53913264	-26.53953964	-26.53958364
bh3	FC	4	1	8	6	174	383.878	52.436	-26.40216193	-26.54263541	-26.54544460	-26.54582683	-26.54587857
cf	CV	2	2	15	11	36	1.971	1.605	-137.17999475	-137.53908813	-137.54732170	-137.54794583	-137.54858557
cf	CV	3	2	15	11	86	65.735	27.816	-137.22546512	-137.70192845	-137.71627024	-137.71682231	-137.71743168
cf	CV	4	2	15	11	168	1682.503	360.479	-137.23585138	-137.74697926	-137.76282053	-137.76330368	-137.76398383

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
cf	FC	2	2	15	11	36	0.473	0.396	-137.17994603	-137.47885326	-137.48676280	-137.48738208	-137.48799671
cf	FC	3	2	15	11	86	29.481	12.52	-137.22536587	-137.60033757	-137.61394537	-137.61447096	-137.61503755
cf	FC	4	2	15	11	168	744.024	140.005	-137.23573823	-137.63340158	-137.64840164	-137.64885519	-137.64948565
ch	CV	2	2	7	5	23	0.069	0.058	-38.27247979	-38.40996861	-38.41212869	-38.41264187	-38.41271457
ch	CV	3	2	7	5	57	2.034	1.23	-38.28151232	-38.45547206	-38.45929150	-38.45995122	-38.46004043
ch	CV	4	2	7	5	114	37.844	10.936	-38.28380427	-38.46765245	-38.47186059	-38.47251350	-38.47261669
ch	FC	2	2	7	5	23	0.035	0.031	-38.27246075	-38.38078317	-38.38273620	-38.38324161	-38.38330644
ch	FC	3	2	7	5	57	0.983	0.677	-38.28148434	-38.40891888	-38.41233081	-38.41296192	-38.41303995
ch	FC	4	2	7	5	114	15.89	6.358	-38.28377380	-38.41573488	-38.41948526	-38.42010682	-38.42019643
ch2-sing	CV	2	1	8	6	28	0.11	0.086	-38.88086049	-39.05171853	-39.05505552	-39.05577284	-39.05593734
ch2-sing	CV	3	1	8	6	71	4.465	2.046	-38.89254771	-39.10532609	-39.11073858	-39.11159396	-39.11179960
ch2-sing	CV	4	1	8	6	144	116.382	23.954	-38.89520977	-39.11949521	-39.12540448	-39.12624483	-39.12647631
ch2-sing	FC	2	1	8	6	28	0.056	0.044	-38.88081905	-39.02229011	-39.02538898	-39.02608299	-39.02623837
ch2-sing	FC	3	1	8	6	71	2.369	1.188	-38.89248904	-39.05842329	-39.06338823	-39.06417940	-39.06437262
ch2-sing	FC	4	1	8	6	144	59.226	14.272	-38.89514649	-39.06719512	-39.07260444	-39.07337382	-39.07359034
ch2-trip	CV	2	3	8	6	28	0.151	0.12	-38.92690162	-39.07217750	-39.07421846	-39.07459884	-39.07467462
ch2-trip	CV	3	3	8	6	71	5.765	2.58	-38.93793509	-39.12378128	-39.12758543	-39.12807201	-39.12815187
ch2-trip	CV	4	3	8	6	144	157.703	29.687	-38.94028303	-39.13710919	-39.14134081	-39.14181533	-39.14191071
ch2-trip	FC	2	3	8	6	28	0.045	0.037	-38.92688030	-39.04241223	-39.04432104	-39.04469967	-39.04477058
ch2-trip	FC	3	3	8	6	71	2.73	1.485	-38.93791348	-39.07618279	-39.07970186	-39.08017587	-39.08024951
ch2-trip	FC	4	3	8	6	144	70.724	16.622	-38.94026008	-39.08405446	-39.08795594	-39.08841631	-39.08850397
ch3	CV	2	2	9	7	33	0.655	0.524	-39.56397316	-39.74626635	-39.74925885	-39.74966352	-39.74978204
ch3	CV	3	2	9	7	85	32.493	12.223	-39.57777943	-39.80604244	-39.81123495	-39.81170560	-39.81182609
ch3	CV	4	2	9	7	174	1372.48	198.768	-39.58041428	-39.82121774	-39.82692759	-39.82737265	-39.82751443
ch3	FC	2	2	9	7	33	0.332	0.265	-39.56394254	-39.71617973	-39.71901573	-39.71941626	-39.71952853
ch3	FC	3	2	9	7	85	17.693	6.537	-39.57774381	-39.75808656	-39.76295259	-39.76340237	-39.76351681
ch3	FC	4	2	9	7	174	762.804	101.646	-39.58037545	-39.76778568	-39.77311982	-39.77354098	-39.77367545
cn	CV	2	2	13	9	36	1.063	0.915	-92.21288843	-92.54349675	-92.55752528	-92.56023160	-92.56244733
cn	CV	3	2	13	9	86	52.882	25.859	-92.23590032	-92.65022222	-92.67030792	-92.67270090	-92.67515355
cn	CV	4	2	13	9	168	1247.397	300.074	-92.24154595	-92.68032292	-92.70168064	-92.70389156	-92.70644781
cn	FC	2	2	13	9	36	0.363	0.309	-92.21282507	-92.48375212	-92.49727206	-92.49994851	-92.50211314
cn	FC	3	2	13	9	86	19.942	9.416	-92.23574144	-92.55299177	-92.57208287	-92.57437395	-92.57677393
cn	FC	4	2	13	9	168	483.709	108.878	-92.24137441	-92.57182076	-92.59207033	-92.59416845	-92.59666884

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
co	CV	2	1	14	10	36	0.979	0.718	-112.74830388	-113.11309986	-113.12534435	-113.12569583	-113.12683552
co	CV	3	1	14	10	86	36.044	13.122	-112.78112978	-113.24593946	-113.26442684	-113.26454369	-113.26574162
co	CV	4	1	14	10	168	962.525	163.759	-112.78900821	-113.28356208	-113.30335674	-113.30336787	-113.30464938
co	FC	2	1	14	10	36	0.383	0.273	-112.74818495	-113.05298985	-113.06486418	-113.06520763	-113.06631360
co	FC	3	1	14	10	86	15.205	5.459	-112.78084289	-113.14616260	-113.16383012	-113.16389183	-113.16504662
co	FC	4	1	14	10	168	407.744	66.567	-112.78868462	-113.17210120	-113.19096316	-113.19091005	-113.19214366
f2	CV	2	1	18	14	36	1.001	0.582	-198.68080708	-199.16575320	-199.17722624	-199.17740005	-199.17922989
f2	CV	3	1	18	14	86	52.892	15.165	-198.75233363	-199.40073624	-199.42053685	-199.42052303	-199.42216063
f2	CV	4	1	18	14	168	1172.257	155.216	-198.76847319	-199.46628306	-199.48861466	-199.48856261	-199.49034463
f2	FC	2	1	18	14	36	0.548	0.338	-198.68069242	-199.10429413	-199.11535979	-199.11552078	-199.11732619
f2	FC	3	1	18	14	86	26.715	7.496	-198.75216623	-199.29151329	-199.31044115	-199.31037447	-199.31198118
f2	FC	4	1	18	14	168	583.776	71.915	-198.76828689	-199.34390708	-199.36523337	-199.36512083	-199.36686479
h2o	CV	2	1	10	8	28	0.167	0.127	-76.02651910	-76.27485871	-76.27856217	-76.27867957	-76.27915731
h2o	CV	3	1	10	8	71	6.99	2.841	-76.05716368	-76.38175254	-76.39012489	-76.39017779	-76.39055978
h2o	CV	4	1	10	8	144	195.33	34.925	-76.06490106	-76.41156061	-76.42112891	-76.42113016	-76.42156432
h2o	FC	2	1	10	8	28	0.077	0.06	-76.02647141	-76.24405034	-76.24760594	-76.24772403	-76.24819200
h2o	FC	3	1	10	8	71	4.136	1.704	-76.05709849	-76.32901971	-76.33703792	-76.33708150	-76.33744554
h2o	FC	4	1	10	8	144	112.801	20.363	-76.06482927	-76.35263840	-76.36179261	-76.36178278	-76.36219434
h2s	CV	2	1	18	8	37	1.612	1.168	-398.69833424	-399.01922297	-399.02434843	-399.02472062	-399.02499210
h2s	CV	3	1	18	8	87	69.746	22.717	-398.71557366	-399.22631417	-399.23714128	-399.23770457	-399.23813352
h2s	CV	4	1	18	8	169	1795.367	252.554	-398.71936612	-399.31911073	-399.33187877	-399.33242862	-399.33295238
h2s	FC	2	1	18	8	37	0.166	0.112	-398.69833271	-398.86972572	-398.87350560	-398.87395968	-398.87419970
h2s	FC	3	1	18	8	87	7.76	2.636	-398.71554239	-398.93268415	-398.94092557	-398.94161101	-398.94196098
h2s	FC	4	1	18	8	169	214.704	33.078	-398.71932286	-398.94926204	-398.95877038	-398.95943606	-398.95986664
hcl	CV	2	1	18	8	32	0.647	0.458	-460.09151330	-460.41141575	-460.41553822	-460.41574014	-460.41602975
hcl	CV	3	1	18	8	73	29.228	11.679	-460.10816109	-460.63572874	-460.64641303	-460.64678033	-460.64718099
hcl	CV	4	1	18	8	139	665.435	130.431	-460.11197306	-460.73315290	-460.74604615	-460.74642237	-460.74693061
hcl	FC	2	1	18	8	32	0.071	0.056	-460.09150769	-460.26153724	-460.26447810	-460.26475676	-460.26501459
hcl	FC	3	1	18	8	73	3.546	1.44	-460.10814486	-460.33509940	-460.34335379	-460.34386112	-460.34418343
hcl	FC	4	1	18	8	139	79.548	14.671	-460.11194986	-460.35610308	-460.36593633	-460.36645000	-460.36686127
hf	CV	2	1	10	8	23	0.068	0.054	-100.01948288	-100.26530506	-100.26781600	-100.26786534	-100.26826447
hf	CV	3	1	10	8	57	2.585	1.257	-100.05812315	-100.39349126	-100.40057574	-100.40056650	-100.40083575
hf	CV	4	1	10	8	114	57.219	13.225	-100.06778603	-100.42984437	-100.43824776	-100.43819864	-100.43850711
hf	FC	2	1	10	8	23	0.037	0.031	-100.01946810	-100.23425097	-100.23663890	-100.23669014	-100.23708029

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
hf	FC	3	1	10	8	57	1.524	0.744	-100.05810038	-100.33844122	-100.34520500	-100.34519977	-100.34544893
hf	FC	4	1	10	8	114	33.987	8.094	-100.06775946	-100.36818678	-100.37620836	-100.37616486	-100.37644774
hs	CV	2	2	17	7	32	0.969	0.747	-398.09109313	-398.37845091	-398.38228320	-398.38265948	-398.38284517
hs	CV	3	2	17	7	73	40.607	18.75	-398.10652679	-398.57838940	-398.58735011	-398.58804266	-398.58834457
hs	CV	4	2	17	7	139	835.436	195.554	-398.11010980	-398.66899422	-398.67972819	-398.68043486	-398.68081851
hs	FC	2	2	17	7	32	0.115	0.091	-398.09109061	-398.22903661	-398.23162094	-398.23207084	-398.23222810
hs	FC	3	2	17	7	73	3.904	1.838	-398.10650723	-398.28503150	-398.29150152	-398.29231651	-398.29253950
hs	FC	4	2	17	7	139	85.997	17.741	-398.11008442	-398.29940528	-398.30697871	-398.30780459	-398.30809405
n2	CV	2	1	14	10	36	0.609	0.353	-108.95116256	-109.33300576	-109.34677366	-109.34668263	-109.34852712
n2	CV	3	1	14	10	86	25.24	6.669	-108.98396469	-109.46250103	-109.48266269	-109.48237827	-109.48425087
n2	CV	4	1	14	10	168	549.429	64.053	-108.99122856	-109.49830823	-109.51983923	-109.51946077	-109.52143528
n2	FC	2	1	14	10	36	0.27	0.149	-108.95101066	-109.27250362	-109.28585392	-109.28575323	-109.28756761
n2	FC	3	1	14	10	86	11.017	2.741	-108.98359101	-109.36244705	-109.38171605	-109.38135392	-109.38320136
n2	FC	4	1	14	10	168	240.991	27.613	-108.99080184	-109.38663124	-109.40714961	-109.40667935	-109.40862684
nh	CV	2	3	8	6	23	0.076	0.062	-54.96639596	-55.12410627	-55.12596435	-55.12624625	-55.12636256
nh	CV	3	3	8	6	57	2.46	1.436	-54.98134565	-55.18942887	-55.19370750	-55.19414752	-55.19425762
nh	CV	4	3	8	6	114	49.55	13.312	-54.98518536	-55.20660006	-55.21150381	-55.21194847	-55.21208092
nh	FC	2	3	8	6	23	0.04	0.035	-54.96637362	-55.09402344	-55.09575383	-55.09603580	-55.09614619
nh	FC	3	3	8	6	57	1.255	0.814	-54.98131792	-55.13973877	-55.14371319	-55.14414606	-55.14424547
nh	FC	4	3	8	6	114	22.054	7.149	-54.98515471	-55.15115858	-55.15570819	-55.15614463	-55.15626328
nh2	CV	2	2	9	7	28	0.23	0.187	-55.56679391	-55.76480231	-55.76792832	-55.76825451	-55.76847970
nh2	CV	3	2	9	7	71	8.266	3.925	-55.58611559	-55.84086933	-55.84708221	-55.84748702	-55.84769754
nh2	CV	4	2	9	7	144	218.42	44.785	-55.59074032	-55.86115163	-55.86814954	-55.86853637	-55.86878077
nh2	FC	2	2	9	7	28	0.131	0.106	-55.56674362	-55.73442696	-55.73740250	-55.73772781	-55.73794556
nh2	FC	3	2	9	7	71	4.628	2.277	-55.58605125	-55.79084982	-55.79672118	-55.79711040	-55.79730975
nh2	FC	4	2	9	7	144	123.969	25.811	-55.59067050	-55.80535514	-55.81195771	-55.81232633	-55.81255642
nh3	CV	2	1	10	8	33	0.958	0.785	-56.19535618	-56.43370142	-56.43817777	-56.43841900	-56.43875753
nh3	CV	3	1	10	8	85	65.689	25.399	-56.21799275	-56.51893974	-56.52722468	-56.52743334	-56.52775149
nh3	CV	4	1	10	8	174	3366.784	513.298	-56.22320010	-56.54170756	-56.55092847	-56.55108800	-56.55145221
nh3	FC	2	1	10	8	33	0.502	0.411	-56.19527476	-56.40295182	-56.40726796	-56.40750683	-56.40783625
nh3	FC	3	1	10	8	85	38.524	14.053	-56.21789415	-56.46843014	-56.47635857	-56.47654302	-56.47684980
nh3	FC	4	1	10	8	174	1937.267	253.31	-56.22309553	-56.48538175	-56.49419062	-56.49432124	-56.49467120
no	CV	2	2	15	11	36	1.893	1.467	-129.25958504	-129.65750430	-129.67000340	-129.67061441	-129.67215316
no	CV	3	2	15	11	86	65.977	28.769	-129.29727568	-129.80861184	-129.82863013	-129.82891780	-129.83051457

System	CV	Cardinal	M	N _{el}	N _{val_el}	Basis size	Time SDT(Q), min	Time SDT, min	HF	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
no	CV	4	2	15	11	168	1697.14	401.9	-129.30695472	-129.85135411	-129.87305229	-129.87323754	-129.87494742
no	FC	2	2	15	11	36	0.809	0.647	-129.25949207	-129.59681609	-129.60891776	-129.60953310	-129.61103976
no	FC	3	2	15	11	86	30.386	12.623	-129.29707159	-129.70642881	-129.72557437	-129.72581877	-129.72737744
no	FC	4	2	15	11	168	737.902	154.447	-129.30672074	-129.73722703	-129.75793218	-129.75806387	-129.75973079
o2	CV	2	3	16	12	36	1.258	0.806	-149.62693033	-150.04846551	-150.05969467	-150.05976957	-150.06172282
o2	CV	3	3	16	12	86	53.462	15.335	-149.67539619	-150.22515634	-150.24466117	-150.24462170	-150.24653726
o2	CV	4	3	16	12	168	1131.377	141.323	-149.68794573	-150.27459925	-150.29599286	-150.29592850	-150.29794234
o2	FC	2	3	16	12	36	0.559	0.343	-149.62675227	-149.98759933	-149.99848887	-149.99856111	-150.00049335
o2	FC	3	3	16	12	86	24.84	6.767	-149.67508494	-150.12060509	-150.13931898	-150.13922292	-150.14111799
o2	FC	4	3	16	12	168	538.516	63.851	-149.68761250	-150.15773239	-150.17821456	-150.17808220	-150.18007117
oh	CV	2	2	9	7	23	0.108	0.092	-75.39376837	-75.59392703	-75.59611789	-75.59629032	-75.59654034
oh	CV	3	2	9	7	57	3.372	1.9	-75.41935974	-75.68954809	-75.69525634	-75.69553351	-75.69572946
oh	CV	4	2	9	7	114	69.434	18.992	-75.42597524	-75.71589810	-75.72258768	-75.72286496	-75.72309702
oh	FC	2	2	9	7	23	0.054	0.046	-75.39374842	-75.56343659	-75.56549705	-75.56567015	-75.56591309
oh	FC	3	2	9	7	57	1.93	1.084	-75.41933260	-75.63717770	-75.64256132	-75.64283474	-75.64301563
oh	FC	4	2	9	7	114	39.853	10.906	-75.42594425	-75.65736459	-75.66367243	-75.66394543	-75.66415793
sih	CV	2	2	15	5	32	1.008	0.826	-289.43070478	-289.66230706	-289.66563352	-289.66614179	-289.66619823
sih	CV	3	2	15	5	73	31.058	14.264	-289.44000027	-289.82949217	-289.83549425	-289.83620858	-289.83637461
sih	CV	4	2	15	5	139	590.636	133.256	-289.44242225	-289.90581093	-289.91296800	-289.91366301	-289.91385717
sih	FC	2	2	15	5	32	0.068	0.057	-289.43071043	-289.52115900	-289.52292606	-289.52349059	-289.52353716
sih	FC	3	2	15	5	73	1.89	1.155	-289.43998824	-289.54520485	-289.54828012	-289.54906897	-289.54915069
sih	FC	4	2	15	5	139	35.813	11.225	-289.44240827	-289.55135979	-289.55480295	-289.55557140	-289.55567039