

Benchmarking of Density Functional Theories for Combustion Reactions in Alkanes by Evaluating Thermodynamic Properties

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Supplementary Data

Thermochemistry data for alkane combustion

Table S1: LSDA_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-182.28185	-166.29871	-0.0536077
2	-320.64005	-301.83914	-0.0630585
3	-456.26355	-434.90029	-0.0716527
4	-592.21462	-568.37621	-0.0799544
5	-727.80800	-701.38841	-0.0886117
6	-865.20422	-836.60443	-0.0959242
7	-1001.2883	-970.22656	-0.1041816
8	-1136.7719	-1103.3693	-0.1120329
9	-1272.4067	-1236.9262	-0.1190023
10	-1408.1563	-1370.3751	-0.1267188

Table S2: PBEPBE_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-164.30747	-148.74350	-0.0522018
2	-294.51149	-276.52353	-0.0603319
3	-422.92523	-402.79690	-0.0675107
4	-552.12523	-529.86909	-0.0746475
5	-680.61552	-656.17886	-0.0819610
7	-940.77695	-912.18382	-0.0959018
8	-1069.9512	-1039.3552	-0.1026197
9	-1199.1305	-1166.5516	-0.1092703
10	-1328.3851	-1293.8083	-0.1159713

Table S3: TPSSh_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-159.68335	-144.10244	-0.0522586
2	-287.61046	-269.58735	-0.0604498
3	-414.12001	-393.91827	-0.0677570
4	-541.43780	-519.09068	-0.0749526
5	-668.02015	-643.47368	-0.0823293
7	-924.49308	-895.76001	-0.0963712
8	-1051.8786	-1021.0993	-0.1032343
9	-1179.1876	-1146.4042	-0.1099564
10	-1306.5563	-1271.5847	-0.1172951

Table S4: B3LYP_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-169.13176	-153.53705	-0.0523049
2	-303.65807	-285.61457	-0.0605182
3	-436.64447	-416.43707	-0.0677759
4	-570.52820	-548.20398	-0.0748758
5	-703.61939	-679.11434	-0.0821904
6	-839.19301	-812.54289	-0.0893850
7	-973.26751	-944.53758	-0.0963607
8	-1107.2510	-1076.5116	-0.1031006
9	-1241.1724	-1208.4015	-0.1099143
10	-1375.1735	-1340.3434	-0.1168205

Table S5: B2PLYP_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-173.86507	-158.25152	-0.0523681
2	-311.78651	-293.72827	-0.0605677
3	-447.74260	-427.53019	-0.0677928
4	-584.49751	-562.16356	-0.0749084
5	-720.49187	-695.98493	-0.0821967
6	-858.92411	-832.38725	-0.0890051
7	-995.80577	-967.19632	-0.0959566
8	-1132.5130	-1101.9244	-0.1025945
9	-1269.1763	-1236.6651	-0.1090430
10	-1405.9036	-1371.2608	-0.1161923

Table S6: B2PLYPD3_6-31G(d)

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-173.87197	-158.25968	-0.0523639
2	-311.26443	-293.20932	-0.0605571
3	-446.38781	-426.18292	-0.0677675
4	-582.10858	-559.79157	-0.0748516
5	-717.17799	-692.68925	-0.0821356
6	-854.42236	-827.98150	-0.0886830
7	-990.19395	-961.69181	-0.0955967
8	-1125.6236	-1095.1806	-0.1021062
9	-1261.0651	-1228.7836	-0.1082726
10	-1396.5825	-1362.1808	-0.1153841

Table S7: LSDA_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-191.59284	-175.59526	-0.0536561
2	-334.85188	-316.02839	-0.0631343
3	-475.26266	-453.89437	-0.0716696
4	-616.12461	-592.19961	-0.0802448
5	-756.59249	-730.08254	-0.0889148
6	-898.83183	-870.03625	-0.0965808
7	-1039.8538	-1008.5442	-0.1050130
8	-1180.1711	-1146.5175	-0.1128748
9	-1320.7456	-1284.9256	-0.1201409
10	-1461.4369	-1423.0577	-0.1287246

Table S8: PBEPBE_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-173.59900	-158.01558	-0.0522671
2	-308.61288	-290.60264	-0.0604066
3	-441.76871	-421.61026	-0.0676118
4	-575.80054	-553.47443	-0.0748821
5	-709.11387	-684.60818	-0.0821925
6	-844.68058	-818.04301	-0.0893429
7	-978.90882	-950.12304	-0.0965480
8	-1112.9306	-1082.1202	-0.1033385
9	-1246.9468	-1214.0892	-0.1102047
10	-1381.0708	-1346.2188	-0.1168942

Table S9: TPSSh_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-168.08006	-152.48785	-0.0522965
2	-300.31062	-282.28908	-0.0604445
3	-431.08724	-410.89930	-0.0677107
4	-562.76120	-540.38992	-0.0750337
5	-693.67023	-669.10619	-0.0823882
6	-826.99831	-800.25657	-0.0896922
7	-958.85362	-929.99442	-0.0967942
8	-1090.5847	-1059.6413	-0.1037847
9	-1222.2599	-1189.2574	-0.1106909
10	-1354.0198	-1318.9495	-0.1176266

Table S10: B3LYP_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-177.98906	-162.37928	-0.0523555
2	-316.94025	-298.88985	-0.0605413
3	-454.27623	-434.07260	-0.0677633
4	-592.61434	-570.24494	-0.0750273
5	-730.13293	-705.58457	-0.0823356
6	-872.86862	-847.35868	-0.0855608
7	-1008.6553	-979.82620	-0.0966932
8	-1147.1032	-1116.2345	-0.1035342
9	-1285.4746	-1252.5857	-0.1103100
10	-1423.9438	-1388.9783	-0.1172751

Table S11: B2PLYP_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol.K)
1	-183.22061	-167.18475	-0.0537845
2	-325.90140	-307.01766	-0.0633364
3	-466.60742	-445.13936	-0.0720042
4	-608.15995	-584.14333	-0.0805521
5	-748.94252	-722.33782	-0.0892326
6	-892.12532	-863.07623	-0.0974311
7	-1033.8234	-1002.2791	-0.1058001
8	-1175.3132	-1141.3389	-0.1139503
9	-1316.7628	-1280.4515	-0.1217889
10	-1458.2959	-1419.4755	-0.1302042

Table S12: B2PLYPD3_cc-pVDZ

No. of C atom	Reaction Enthalpy (kcal/mol)	Gibbs Free Energy Change (kcal/mol)	Entropy (kcal/mol ⁻¹ ΣK)
1	-183.22688	-167.19102	-0.0537845
2	-325.38119	-306.49809	-0.0633343
3	-465.25765	-443.79398	-0.0719895
4	-605.77918	-581.77637	-0.0805058
5	-745.63994	-719.04967	-0.0891842
6	-887.63926	-858.67362	-0.0971512
7	-1028.2348	-996.78465	-0.1054844
8	-1168.4457	-1134.6001	-0.1135188
9	-1308.6761	-1272.5800	-0.1210670
10	-1448.9918	-1410.4639	-0.1292234

Scale factor for enthalpy change

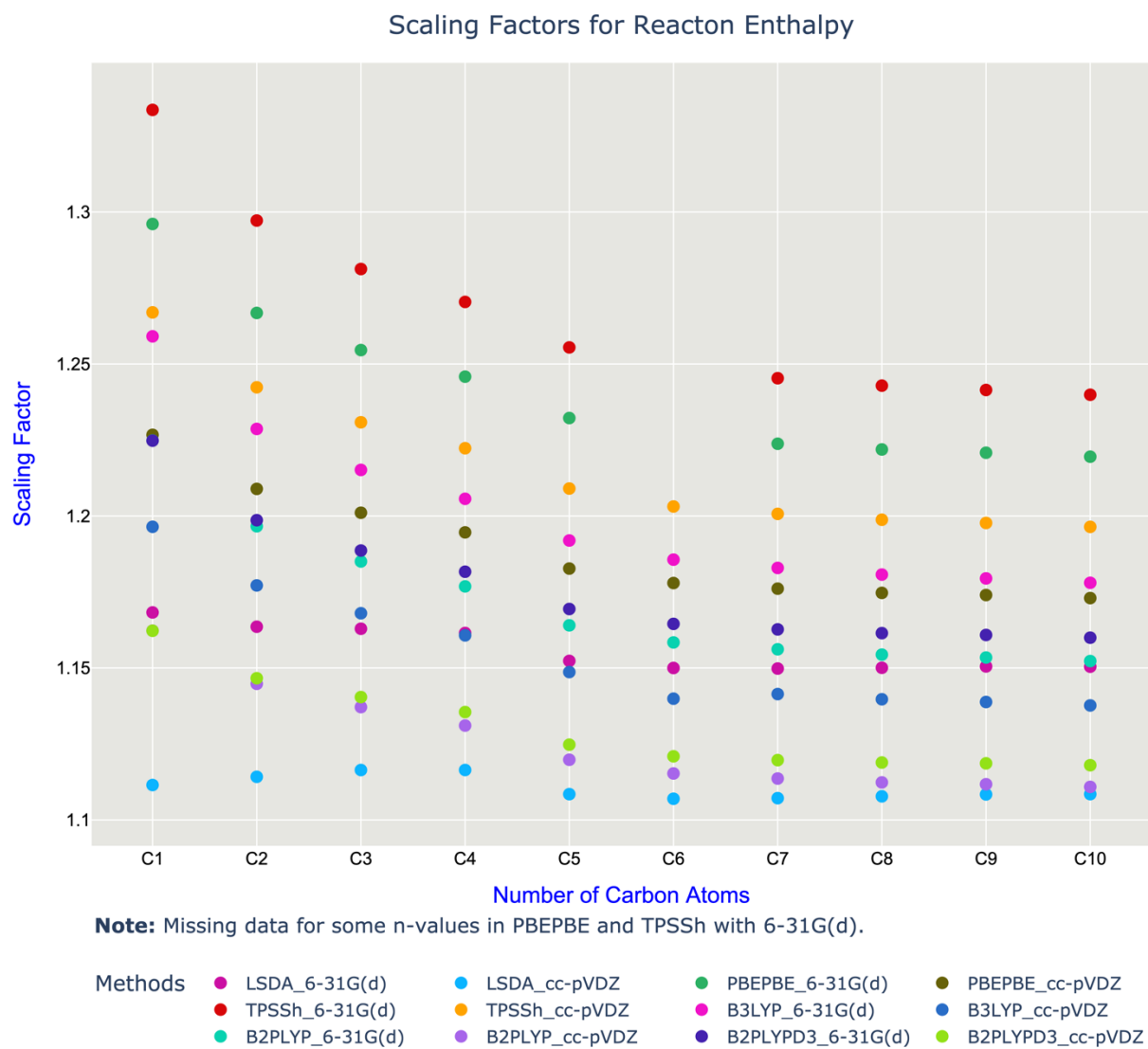


Figure S1: Scale factors for DFT methods for enthalpy

Link for Python Codes

https://github.com/kfatema10/alkane_combustion