Electronic supporting information for:

Computational Thermochemistry: Scale Factor Databases and Scale Factors for Vibrational Frequencies Obtained from Electronic Model Chemistries

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Table S1. Summary of previous scale factors for electronic model chemistries.

Model chemistry	λ^Y	N[a]	Ref.	Method
AM1	0.9532	F	2	2
B1B95/6-31+G(d,p)	0.9735	ZPE	6	3
B1B95/MG3S	0.9758	ZPE	6	3
B3LYP/6-31G(2df,2p)	0.9830	ZPE	9	3
B3LYP/6-31G(d)	0.9806	ZPE	2	2
B3LYP/MG3S	0.9853	ZPE	11	3
B3LYP/MG3S	0.9983	H	11	11
B3P86/6-31G(d)	0.9759	ZPE	2	2
B3PW91/6-31G(d)	0.9772	ZPE	2	2
B97-3/MG3S	0.9743	ZPE	11	3
B97-3/MG3S	0.9856	H	11	11
B98/MG3S	0.9844	ZPE	11	3
B98/MG3S	0.9954	H	11	11
BB1K/6-31+G(d,p)	0.9561	ZPE	6	3
BB1K/MG3S	0.9590	ZPE	6	3
BB95/6-31+G(d,p)	1.0139	ZPE	6	3
BB95/MG3S	1.0144	ZPE	6	3
BLYP/6-311G(df,p)	1.0167	ZPE	2	2
BLYP/6-31G(d)	1.0126	ZPE	2	2
BLYP/MG3S	1.0156	ZPE	11	3
BLYP/MG3S	1.0307	H	11	11
BMK/MG3S	0.9734	ZPE	11	3
BMK/MG3S	0.9835	H	11	11
BP86/6-31G(d)	1.0108	ZPE	2	2
BPW60/6-311+G(d,p)	0.9363	ZPE	5	3
BPW63/MG3S	0.9252	ZPE	5	3
G96LYP80/6-311+G(d,p)	0.9135	ZPE	5	3
G96LYP82/MG3S	0.9094	ZPE	5	3
HF/3-21G	0.9207	ZPE	2	2

Table S1. Continued.

Model chemistry	λ^{Y}	N[a]	Ref.	Method
HF/6-31+G(d)	0.9163	ZPE	2	2
HF/6-31+G(d,p)	0.9173	ZPE	6	3
HF/6-311G(d,p)	0.9248	ZPE	2	2
HF/6-311G(df,p)	0.9247	ZPE	2	2
HF/6-31G(d)	0.9135	ZPE	1	1
HF/6-31G(d)	0.9135	ZPE	2	2
HF/6-31G(d,p)	0.9181	ZPE	2	2
HF/MG3S	0.9210	ZPE	6	3
HF/MG3S	0.9209	ZPE	11	3
HF/MG3S	0.9323	H	11	11
HFLYP/MG3S	0.9016	ZPE	11	3
HFLYP/MG3S	0.9119	H	11	11
M05-2X/MG3S	0.9642	ZPE	11	3
M05-2X/MG3S	0.9748	H	11	11
M05/MG3S	0.9789	ZPE	11	3
M05/MG3S	0.9894	H	11	11
M06-2X/MG3S	0.9721	ZPE	11	3
M06-2X/MG3S	0.9824	H	11	11
M06-HF/MG3S	0.9570	ZPE	11	3
M06-HF/MG3S	0.9672	H	11	11
M06-L/MG3S	0.9800	ZPE	11	3
M06-L/MG3S	0.9964	H	11	11
M06/MG3S	0.9830	ZPE	11	3
M06/MG3S	0.9939	H	11	11
M08-HX/cc-pVTZ+	0.9761	ZPE	12	3
MC3BB	0.9675	ZPE	7	3
MC3MPW	0.9669	ZPE	7	3
MC-QCISD/3	0.9940	ZPE	7	3
MP2(FC)/6-31+G(d,p)	0.9700	ZPE	7	3

Table S1. Continued.

Model chemistry	λ^{Y}	N[a]	Ref.	Method
MP2(FC)/6-311G(d,p)	0.9748	ZPE	2	2
MP2(FC)/6-31G(d)	0.9670	ZPE	2	2
MP2(FC)/6-31G(d,p)	0.9608	ZPE	2	2
MP2(FC)/cc-pVDZ	0.9790	ZPE	3	3
MP2(FULL)/6-31G(d)	0.9646	ZPE	1	1
MPW1B95/6-31+G(d,p)	0.9721	ZPE	8	3
MPW1B95/MG3	0.9722	ZPE	10	3
MPW1B95/MG3S	0.9746	ZPE	8	3
MPW1K/6-31+G(d,p)	0.9515	ZPE	4	3
MPW1K/MG3	0.9552	ZPE	4	3
MPW1K/MG3S	0.9581	ZPE	6	3
MPW3LYP/6-31+G(d,p)	0.9825	ZPE	8	3
MPW3LYP/MG3S	0.9846	ZPE	8	3
MPW74/6-311+G(d,p)	0.9147	ZPE	5	3
MPW76/MG3S	0.9117	ZPE	5	3
MPWB1K/6-31+G(d,p)	0.9537	ZPE	8	3
MPWB1K/MG3S	0.9567	ZPE	8	3
PBE/MG3S	1.0122	ZPE	11	3
PBE/MG3S	1.0248	H	11	11
PBE1KCIS/MG3	0.9833	ZPE	10	3
PBE1KCIS/MG3S	0.9832	ZPE	10	3
PBE0/MG3S	0.9779	ZPE	11	3
PBE0/MG3S	0.9887	H	11	11
PM3	0.9761	F	2	2
PM6	0.9860	F	13	2
PW6B95/6-31+G(d,p)	0.9720	ZPE	10	3
QCISD(FC)/6-31G(d)	0.9776	ZPE	2	2
TPSSh/MG3S	0.9864	ZPE	11	3
TPSSh/MG3S	1.0016	H	11	11

Table S1. Continued.

Model chemistry	λ^Y	N[a]	Ref.	Method
VSXC/MG3S	0.9885	ZPE	11	3
VSXC/MG3S	1.0014	H	11	11
X1B95/6-31+G(d,p)	0.9709	ZPE	8	3
X1B95/MG3S	0.9733	ZPE	8	3
XB1K/6-31+G(d,p)	0.9549	ZPE	8	3
XB1K/MG3S	0.9579	ZPE	8	3

[a] F, H, and ZPE refer to fundamental frequencies, harmonic frequencies, and zero-point vibrational energy, respectively.

Table S2. Absolute ZPE deviations for new scale factors in kcal mol^{-1} and as a percentage for diatomic species.

Model	HF		H_2		OH		N_2		CO		F_2		Cl_2		Average[b]	
chemistry[a]	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%
B1LYP/MG3S	0.027	0.4	0.104	1.8	0.071	1.3	0.082	2.4	0.023	0.7	0.177	13.6	0.043	5.4	0.108	2.3
B3LYP/MG3S	0.019	0.3	0.109	1.9	0.077	1.4	0.073	2.2	0.018	0.6	0.166	12.8	0.045	5.6	0.102	2.2
B97-3/MG3S	0.032	0.5	0.036	0.6	0.028	0.5	0.080	2.4	0.024	0.8	0.209	16.0	0.015	1.9	0.095	2.0
B98/MG3S	0.003	0.0	0.030	0.5	0.023	0.4	0.061	1.8	0.023	0.8	0.203	15.6	0.018	2.2	0.078	1.8
BLYP/MG3S	0.067	1.1	0.160	2.7	0.128	2.4	0.011	0.3	0.029	0.9	0.081	6.2	0.074	9.3	0.086	2.0
BMC-CCSD	0.079	1.3	0.011	0.2	0.040	0.8	0.057	1.7	0.030	1.0	0.026	2.0	0.017	2.1	0.081	1.1
BMK/MG3S	0.004	0.1	0.024	0.4	0.001	0.0	0.025	0.8	0.081	2.6	0.256	19.6	0.050	6.2	0.096	2.4
HF/MG3S	0.205	3.3	0.032	0.5	0.030	0.6	0.221	6.6	0.096	3.1	0.359	27.6	0.002	0.3	0.214	3.9
HFLYP/MG3S	0.232	3.7	0.018	0.3	0.045	0.9	0.222	6.6	0.104	3.4	0.397	30.5	0.029	3.6	0.232	4.5
M05-2X/DIDZ	0.033	0.5	0.153	2.6	0.075	1.4	0.157	4.7	0.036	1.1	0.303	23.3	0.061	7.6	0.157	3.6
M05-2X/def2	0.007	0.1	0.150	2.6	0.076	1.4	0.147	4.4	0.050	1.6	0.327	25.1	0.016	2.0	0.174	3.4
M05-2X/MG3S	0.014	0.2	0.125	2.1	0.067	1.3	0.137	4.1	0.041	1.3	0.318	24.5	0.025	3.1	0.163	3.3
M05/MG3S	0.121	1.9	0.038	0.6	0.015	0.3	0.028	0.8	0.010	0.3	0.216	16.6	0.036	4.5	0.110	2.4
M06-2X/DIDZ	0.079	1.3	0.092	1.6	0.063	1.2	0.154	4.6	0.057	1.9	0.284	21.8	0.036	4.5	0.148	3.2
M06-2X/AVTZ	0.028	0.5	0.086	1.5	0.057	1.1	0.141	4.2	0.062	2.0	0.316	24.3	0.001	0.1	0.158	3.1
M06-2X/def2	0.037	0.6	0.079	1.4	0.052	1.0	0.144	4.3	0.069	2.2	0.312	24.0	0.004	0.5	0.162	3.1
M06-2X/maug	0.030	0.5	0.075	1.3	0.050	0.9	0.141	4.2	0.061	2.0	0.316	24.3	0.010	1.3	0.155	3.1
M06-2X/MG3S	0.031	0.5	0.060	1.0	0.037	0.7	0.133	4.0	0.067	2.2	0.307	23.5	0.002	0.3	0.149	2.9
M06-HF/DIDZ	0.040	0.6	0.250	4.3	0.130	2.5	0.247	7.3	0.122	3.9	0.387	29.7	0.075	9.4	0.240	5.0
M06-HF/def2	0.098	1.6	0.219	3.7	0.076	1.4	0.241	7.2	0.133	4.3	0.418	32.1	0.021	2.6	0.246	4.7
M06-HF/MG3S	0.109	1.7	0.250	4.3	0.102	1.9	0.221	6.6	0.110	3.5	0.398	30.5	0.040	5.0	0.248	4.8
M06-L/DIDZ	0.079	1.3	0.042	0.7	0.036	0.7	0.026	0.8	0.029	0.9	0.051	3.9	0.034	4.2	0.081	1.3
M06-L/def2	0.189	3.0	0.075	1.3	0.059	1.1	0.020	0.6	0.021	0.7	0.073	5.6	0.007	0.8	0.077	1.3
M06-L/MG3S	0.189	3.0	0.037	0.6	0.062	1.2	0.002	0.1	0.012	0.4	0.065	5.0	0.001	0.1	0.071	1.1
M06/DIDZ	0.002	0.0	0.042	0.7	0.003	0.1	0.085	2.5	0.013	0.4	0.170	13.1	0.019	2.4	0.099	1.9
M06/def2	0.211	3.4	0.051	0.9	0.002	0.0	0.091	2.7	0.036	1.2	0.197	15.1	0.006	0.8	0.146	2.5
M06/MG3S	0.202	3.2	0.071	1.2	0.001	0.0	0.079	2.3	0.044	1.4	0.193	14.8	0.002	0.2	0.139	2.4
M08-HX/DIDZ	0.027	0.4	0.137	2.3	0.012	0.2	0.189	5.6	0.093	3.0	0.284	21.8	0.037	4.6	0.135	3.2
M08-HX/VTZ+	0.052	0.8	0.144	2.5	0.003	0.1	0.181	5.4	0.090	2.9	0.312	23.9	0.019	2.4	0.149	3.2

Table S2. Continued.

Model chemistry[a]	HF		H_2		OH		N_2		CO		F_2		Cl_2		Average [b]	
	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%
M08-HX/def2	0.057	0.9	0.123	2.1	0.002	0.0	0.187	5.5	0.101	3.3	0.307	23.6	0.014	1.7	0.148	3.2
M08-HX/MG3S	0.045	0.7	0.113	1.9	0.001	0.0	0.170	5.0	0.092	3.0	0.297	22.8	0.004	0.5	0.140	3.0
M08-SO/DIDZ	0.020	0.3	0.052	0.9	0.042	0.8	0.153	4.6	0.056	1.8	0.257	19.8	0.025	3.1	0.137	2.8
M08-SO/ VTZ+	0.143	2.3	0.037	0.6	0.049	0.9	0.158	4.7	0.079	2.6	0.287	22.1	0.023	2.9	0.159	3.2
M08-SO/def2	0.155	2.5	0.038	0.7	0.036	0.7	0.160	4.8	0.079	2.6	0.281	21.6	0.017	2.1	0.164	3.2
M08-SO/MG3S	0.141	2.3	0.012	0.2	0.032	0.6	0.149	4.4	0.08	2.6	0.276	21.2	0.011	1.4	0.152	3.0
M08-SO/MSXP	0.134	2.2	0.003	0.1	0.018	0.3	0.158	4.7	0.088	2.9	0.279	21.4	0.016	2.0	0.156	3.1
PBE/MG3S	0.002	0.0	0.108	1.8	0.081	1.5	0.026	0.8	0.019	0.6	0.130	10.0	0.027	3.3	0.072	1.6
PBE0/MG3S	0.082	1.3	0.050	0.9	0.024	0.5	0.094	2.8	0.031	1.0	0.223	17.1	0.001	0.1	0.109	2.2
TPSSh/MG3S	0.022	0.3	0.146	2.5	0.107	2.0	0.039	1.2	0.020	0.7	0.156	12.0	0.031	3.9	0.099	2.0
VSXC/MG3S	0.012	0.2	0.080	1.4	0.054	1.0	0.013	0.4	0.041	1.3	0.071	5.5	0.065	8.2	0.067	1.6
Average	0.077	1.2	0.087	1.5	0.047	0.9	0.118	3.5	0.057	1.8	0.242	18.6	0.024	3.1	0.138	2.8
Standard Dev	0.069	1.1	0.063	1.1	0.034	0.6	0.071	2.1	0.034	1.1	0.103	7.9	0.020	2.5	0.049	1.0

[a] The basis sets 6-31+G(d,p), def2-TZVPP, cc-pVTZ+, aug-cc-pVTZ, maug-cc-pV(T+d), and MG3SXP have been abbreviated as DIDZ, def2, VTZ+, AVTZ, maug, and MSXP, respectively.

[b] These absolute and relative deviation values represent the averages for all fifteen (diatomic and polyatomic) ZPEs.

Table S3. Absolute ZPE deviations for new scale factors in kcal mol^{-1} and as a percentage for polyatomic species.

Model	CH_4		NH_3		C_2H_2		H_2CO		H_2O		HCN		CO_2		N_2O	
chemistry[a]	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%
B1LYP/MG3S	0.204	0.7	0.071	0.3	0.165	1.0	0.318	2.0	0.083	0.6	0.047	0.5	0.079	1.1	0.127	1.9
B3LYP/MG3S	0.178	0.6	0.062	0.3	0.151	0.9	0.298	1.9	0.088	0.7	0.037	0.4	0.086	1.2	0.122	1.8
B97-3/MG3S	0.273	1.0	0.043	0.2	0.124	0.8	0.303	1.9	0.007	0.1	0.022	0.2	0.048	0.7	0.186	2.8
B98/MG3S	0.236	0.9	0.022	0.1	0.076	0.5	0.292	1.8	0.018	0.1	0.008	0.1	0.054	0.7	0.105	1.5
BLYP/MG3S	0.013	0.0	0.010	0.0	0.088	0.5	0.207	1.3	0.143	1.1	0.016	0.2	0.199	2.7	0.058	0.9
BMC-CCSD	0.117	0.4	0.023	0.1	0.098	0.6	0.466	2.9	0.024	0.2	0.141	1.4	0.085	1.2	0.000	0.0
BMK/MG3S	0.348	1.3	0.045	0.2	0.018	0.1	0.399	2.5	0.062	0.5	0.006	0.1	0.091	1.2	0.032	0.5
HF/MG3S	0.638	2.3	0.133	0.6	0.308	1.9	0.490	3.1	0.058	0.4	0.187	1.9	0.097	1.3	0.359	5.3
HFLYP/MG3S	0.628	2.3	0.188	0.9	0.310	1.9	0.512	3.2	0.031	0.2	0.178	1.8	0.124	1.7	0.459	6.8
M05-2X/DIDZ	0.215	0.8	0.100	0.5	0.108	0.7	0.496	3.1	0.204	1.5	0.083	0.8	0.148	2.0	0.181	2.7
M05-2X/def2	0.269	1.0	0.192	0.9	0.235	1.4	0.475	3.0	0.222	1.7	0.095	1.0	0.061	0.8	0.289	4.3
M05-2X/MG3S	0.251	0.9	0.191	0.9	0.170	1.0	0.492	3.1	0.190	1.4	0.078	0.8	0.066	0.9	0.282	4.2
M05/MG3S	0.299	1.1	0.040	0.2	0.055	0.3	0.241	1.5	0.051	0.4	0.027	0.3	0.100	1.4	0.375	5.5
M06-2X/DIDZ	0.278	1.0	0.107	0.5	0.148	0.9	0.407	2.5	0.132	1.0	0.092	0.9	0.095	1.3	0.200	3.0
M06-2X/AVTZ	0.307	1.1	0.185	0.9	0.249	1.5	0.403	2.5	0.120	0.9	0.095	0.9	0.023	0.3	0.291	4.3
M06-2X/def2	0.337	1.2	0.181	0.9	0.279	1.7	0.392	2.4	0.111	0.8	0.109	1.1	0.020	0.3	0.300	4.4
M06-2X/maug	0.314	1.1	0.178	0.8	0.247	1.5	0.405	2.5	0.107	0.8	0.082	0.8	0.023	0.3	0.279	4.1
M06-2X/MG3S	0.330	1.2	0.171	0.8	0.236	1.4	0.388	2.4	0.078	0.6	0.090	0.9	0.013	0.2	0.294	4.3
M06-HF/DIDZ	0.176	0.6	0.377	1.8	0.277	1.7	0.721	4.5	0.360	2.7	0.189	1.9	0.223	3.1	0.023	0.3
M06-HF/def2	0.347	1.3	0.364	1.7	0.368	2.2	0.672	4.2	0.272	2.1	0.137	1.4	0.100	1.4	0.216	3.2
M06-HF/MG3S	0.241	0.9	0.401	1.9	0.292	1.8	0.711	4.4	0.353	2.7	0.155	1.5	0.128	1.8	0.210	3.1
M06-L/DIDZ	0.189	0.7	0.165	0.8	0.065	0.4	0.169	1.0	0.052	0.4	0.062	0.6	0.045	0.6	0.165	2.4
M06-L/def2	0.170	0.6	0.027	0.1	0.138	0.8	0.112	0.7	0.002	0.0	0.005	0.0	0.006	0.1	0.249	3.7
M06-L/MG3S	0.165	0.6	0.035	0.2	0.112	0.7	0.110	0.7	0.022	0.2	0.015	0.1	0.016	0.2	0.218	3.2
M06/DIDZ	0.355	1.3	0.014	0.1	0.072	0.4	0.274	1.7	0.046	0.4	0.051	0.5	0.051	0.7	0.282	4.2
M06/def2	0.373	1.3	0.105	0.5	0.243	1.5	0.173	1.1	0.070	0.5	0.101	1.0	0.127	1.7	0.401	5.9
M06/MG3S	0.345	1.2	0.103	0.5	0.195	1.2	0.171	1.1	0.086	0.7	0.081	0.8	0.137	1.9	0.377	5.6
M08-HX/DIDZ	0.383	1.4	0.084	0.4	0.093	0.6	0.310	1.9	0.006	0.0	0.073	0.7	0.075	1.0	0.226	3.3
M08-HX/VTZ+	0.427	1.5	0.038	0.2	0.260	1.6	0.289	1.8	0.004	0.0	0.089	0.9	0.011	0.1	0.315	4.6

Table S3. Continued.

Model chemistry[a]	CH_4		NH_3		C_2H_2		H_2CO		H_2O		HCN		CO_2		N_2O	
	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%	Dev	%
M08-HX/def2	0.424	1.5	0.036	0.2	0.227	1.4	0.275	1.7	0.010	0.1	0.092	0.9	0.008	0.1	0.351	5.2
M08-HX/MG3S	0.416	1.5	0.028	0.1	0.213	1.3	0.264	1.6	0.011	0.1	0.100	1.0	0.005	0.1	0.343	5.1
M08-SO/DIDZ	0.363	1.3	0.085	0.4	0.154	0.9	0.433	2.7	0.062	0.5	0.109	1.1	0.050	0.7	0.201	3.0
M08-SO/ VTZ+	0.415	1.5	0.092	0.4	0.276	1.7	0.340	2.1	0.033	0.2	0.112	1.1	0.029	0.4	0.313	4.6
M08-SO/def2	0.439	1.6	0.101	0.5	0.288	1.7	0.334	2.1	0.014	0.1	0.122	1.2	0.050	0.7	0.341	5.0
M08-SO/MG3S	0.408	1.5	0.107	0.5	0.234	1.4	0.344	2.1	0.006	0.0	0.109	1.1	0.05	0.7	0.326	4.8
M08-SO/MSXP	0.428	1.5	0.114	0.5	0.225	1.4	0.348	2.2	0.008	0.1	0.112	1.1	0.071	1.0	0.345	5.1
PBE/MG3S	0.095	0.3	0.026	0.1	0.063	0.4	0.180	1.1	0.060	0.5	0.017	0.2	0.124	1.7	0.120	1.8
PBE0/MG3S	0.297	1.1	0.043	0.2	0.138	0.8	0.286	1.8	0.010	0.1	0.044	0.4	0.015	0.2	0.291	4.3
TPSSh/MG3S	0.078	0.3	0.071	0.3	0.123	0.7	0.293	1.8	0.145	1.1	0.010	0.1	0.146	2.0	0.093	1.4
VSXC/MG3S	0.129	0.5	0.077	0.4	0.041	0.2	0.159	1.0	0.004	0.0	0.025	0.3	0.138	1.9	0.103	1.5
Average	0.297	1.1	0.111	0.5	0.179	1.1	0.349	2.2	0.084	0.6	0.080	0.8	0.075	1.0	0.236	3.5
Standard Dev	0.134	0.5	0.096	0.5	0.089	0.5	0.148	0.9	0.092	0.7	0.051	0.5	0.054	0.7	0.114	1.7

[a] The basis sets 6-31+G(d,p), def2-TZVPP, cc-pVTZ+, aug-cc-pVTZ, maug-cc-pV(T+d), and MG3SXP have been abbreviated as DIDZ, def2, VTZ+, AVTZ, maug, and MSXP, respectively.

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