Database of Frequency Scale Factors for Electronic Model Chemistries

– Version 4

S. Kanchanakungwankul, J. L. Bao, J. Zheng, I. M. Alecu, B. J. Lynch, Y. Zhao, and D. G. Truhlar

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For thermochemistry and kinetics, use the ZPE scale factor;
and for computing with experimental IR spectra, use the F scale factor.

Model Chemistry	Scale Factor								
	Zero Point Energy (ZPE)			Harmonic Frequencies (H)			Fundamentals (F)		
	Value	Ref.	Method	Value	Ref.	Method	Value	Ref.	Method
AM1	0.948	1	R	0.961	1	R	0.923	1	R
B1B95/6-31+G(d,p)	0.971	1	C	0.985	1	R	0.946	1	R
B1B95/MG3S	0.973	1	C	0.987	1	R	0.948	1	R
B1LYP/MG3S	0.978	1	D	0.994	1	D	0.955	1	D
B3LYP/6-31G(2df,2p)	0.981	1	C	0.995	1	R	0.955	1	R
B3LYP/6-31G(d)	0.977	1	R	0.991	1	R	0.952	1	R
B3LYP/aug-cc-pVTZ	0.985	3	R	0.999	3	R	0.959	3	R
B3LYP/def2-TZVP	0.985	3	R	0.999	3	R	0.959	3	R
B3LYP/ma-TZVP	0.986	1	R	1.000	1	R	0.960	1	R
B3LYP/MG3S	0.983	1	D	0.998	1	D	0.960	1	D
B3P86/6-31G(d)	0.971	1	R	0.985	1	R	0.946	1	R
B3PW91/6-31G(d)	0.972	1	R	0.986	1	R	0.947	1	R
B97-3/def2-TZVP	0.974	8	D	0.988	8	R	0.949	8	R
B97-3/ma-TZVP	0.975	1	R	0.989	1	R	0.950	1	R
B97-3/MG3S	0.972	1	D	0.986	1	D	0.947	1	D
B98/def2-TZVP	0.984	1	R	0.998	1	R	0.958	1	R
B98/ma-TZVP	0.985	1	R	0.999	1	R	0.959	1	R
B98/MG3S	0.982	1	D	0.995	1	D	0.956	1	D
BB1K/6-31+G(d,p)	0.954	1	C	0.967	1	R	0.929	1	R
BB1K/MG3S	0.957	1	C	0.970	1	R	0.932	1	R
BB95/6-31+G(d,p)	1.011	1	C	1.025	1	R	0.985	1	R
BB95/MG3S	1.012	1	C	1.026	1	R	0.986	1	R
BLYP/6-311G(df,p)	1.013	1	R	1.027	1	R	0.987	1	R
BLYP/6-31G(d)	1.009	1	R	1.023	1	R	0.983	1	R
BLYP/MG3S	1.013	1	D	1.031	1	D	0.991	1	D
BMC-CCSD	0.985	1	D	1.001	1	D	0.962	1	D
BMK/ma-TZVP	0.972	1	R	0.986	1	R	0.947	1	R
BMK/MG3S	0.971	1	D	0.984	1	D	0.945	1	D
BP86/6-31G(d)	1.007	1	R	1.021	1	R	0.981	1	R
BP86/ma-TZVP	1.014	1	R	1.028	1	R	0.988	1	R
BPW60/6-311+G(d,p)	0.934	2	C	0.910	2	R	0.947	2	R
BPW63/MG3S	0.923	2	C	0.899	2	R	0.936	2	R
CAM-B3LYP/ma-TZVP	0.976	1	R	0.990	1	R	0.951	1	R

CCSD(T)/jul-cc-pVTZ	0.984	1	R	0.998	1	R	0.958	1	R
CCSD(T)/aug-cc-pVTZ	0.987	1	R	1.001	1	R	0.961	1	R
CCSD(T)-F12/jul-cc-pVTZ	0.981	1	R	0.995	1	R	0.955	1	R
CCSD(T)-F12a/cc-pVDZ-F12	0.983	11	R	0.997	11	R	0.957	11	R
CCSD(T)-F12a/cc-pVTZ-F12	0.984	1	R	0.998	1	R	0.958	1	R
CCSD(T)-F12b/VQZ-F12//CCSD(T)-F12a/TZF	0.984	13	R	0.998	13	R	0.958	13	R
CCSD(T)-F12b/VQZ-F12//CCSD(T)-F12a/DZF	0.983	13	R	0.997	13	R	0.957	13	R
CCSD/jul-cc-pVTZ	0.973	1	R	0.987	1	R	0.948	1	R
CCSD-F12/jul-cc-pVTZ	0.971	1	R	0.985	1	R	0.946	1	R
G96LYP80/6-311+G(d,p)	0.911	2	C	0.887	2	R	0.924	2	R
G96LYP82/MG3S	0.907	2	C	0.883	2	R	0.920	2	R
GAM/def2-TZVP	0.980	7	D	0.994	7	D	0.955	7	D
GAM/ma-TZVP	0.981	7	D	0.995	7	D	0.956	7	D
HF/3-21G	0.919	1	R	0.932	1	R	0.895	1	R
HF/6-31+G(d)	0.911	1	R	0.924	1	R	0.887	1	R
HF/6-31+G(d,p)	0.915	1	C	0.928	1	R	0.891	1	R
HF/6-311G(d,p)	0.920	1	R	0.933	1	R	0.896	1	R
HF/6-311G(df,p)	0.920	1	R	0.933	1	R	0.896	1	R
HF/6-31G(d)	0.909	1	R	0.922	1	R	0.885	1	R
HF/6-31G(d,p)	0.913	1	R	0.926	1	R	0.889	1	R
HF/MG3S	0.919	1	D	0.932	1	D	0.895	1	D
HFLYP/MG3S	0.899	1	D	0.912	1	D	0.876	1	D
HSEh1PBE/ma-TZVP	0.979	1	R	0.993	1	R	0.954	1	R
M05/aug-cc-pVTZ	0.978	1	R	0.992	1	R	0.953	1	R
M05/def2-TZVP	0.978	3	R	0.991	3	R	0.952	3	R
M05/ma-TZVP	0.979	1	R	0.993	1	R	0.954	1	R
M05/maug-cc-pVTZ	0.978	1	R	0.992	1	R	0.953	1	R
M05/MG3S	0.977	1	D	0.989	1	D	0.951	1	D
M05-2X/6-31+G(d,p)	0.961	1	D	0.974	1	D	0.936	1	D
M05-2X/aug-cc-pVTZ	0.964	1	R	0.977	1	R	0.939	1	R
M05-2X/def2-TZVPP	0.962	1	D	0.976	1	D	0.938	1	D
M05-2X/ma-TZVP	0.965	1	R	0.979	1	R	0.940	1	R
M05-2X/maug-cc-pVTZ	0.964	1	R	0.977	1	R	0.939	1	R
M05-2X/MG3S	0.962	1	D	0.975	1	D	0.937	1	D
M06/6-31+G(d,p)	0.980	1	D	0.989	1	D	0.950	1	D
M06/aug-cc-pVTZ	0.984	1	R	0.998	1	R	0.958	1	R
M06/def2-TZVP	0.982	3	R	0.996	3	R	0.956	3	R
M06/def2-TZVPP	0.979	1	D	0.992	1	D	0.953	1	D
M06/ma-TZVP	0.982	1	R	0.996	1	R	0.956	1	R
M06/maug-cc-pVTZ	0.982	1	R	0.996	1	R	0.956	1	R
M06/MG3S	0.981	1	D	0.994	1	D	0.955	1	D
M06-2X/6-31+G(d,p)	0.967	1	D	0.979	1	D	0.940	1	D
M06-2X/6-311+G(d,p)	0.970	5	D	0.983	5	R	0.944	5	R
M06-2X/6-311++G(d,p)	0.970	5	D	0.983	5	R	0.944	5	R

M06-2X/aug-cc-pVDZ	0.979	14	D	0.993	14	R	0.954	14	R
M06-2X/aug-cc-pVTZ	0.971	1	D	0.985	1	D	0.946	1	D
M06-2X/def2-TZVP	0.971	7	D	0.984	7	D	0.946	7	D
M06-2X/def2-QZVP	0.970	7	D	0.983	7	D	0.945	7	D
M06-2X/def2-TZVPP	0.970	1	D	0.983	1	D	0.945	1	D
M06-2X/jul-cc-pVDZ	0.977	14	D	0.991	14	R	0.952	14	R
M06-2X/jul-cc-pVTZ	0.971	14	D	0.985	14	R	0.946	14	R
M06-2X/jun-cc-pVDZ	0.976	14	D	0.990	14	R	0.951	14	R
M06-2X/jun-cc-pVTZ	0.971	14	D	0.985	14	R	0.946	14	R
M06-2X/ma-TZVP	0.972	1	R	0.986	1	R	0.947	1	R
M06-2X/maug-cc-pV(T+d)Z	0.971	1	D	0.984	1	D	0.945	1	D
M06-2X/MG3S	0.970	1	D	0.982	1	D	0.944	1	D
M06-HF/6-31+G(d,p)	0.954	1	D	0.969	1	D	0.931	1	D
M06-HF/aug-cc-pVTZ	0.961	1	R	0.974	1	R	0.936	1	R
M06-HF/def2-TZVPP	0.958	1	D	0.970	1	D	0.932	1	D
M06-HF/ma-TZVP	0.957	1	R	0.970	1	R	0.932	1	R
M06-HF/maug-cc-pVTZ	0.959	1	R	0.972	1	R	0.934	1	R
M06-HF/MG3S	0.955	1	D	0.967	1	D	0.93	1	D
M06-L/6-31G(d,p)	0.977	15	D	0.991	15	R	0.952	15	R
M06-L/6-31+G(d,p)	0.978	1	D	0.992	1	D	0.953	1	D
M06-L/aug-cc-pVTZ	0.980	1	R	0.994	1	R	0.955	1	R
M06-L/aug-cc-pV(T+d)Z	0.980	9	R	0.994	9	R	0.955	9	R
M06-L/aug-cc-pVTZ-pp	0.980	9	R	0.994	9	R	0.955	9	R
M06-L(DKH2)/aug-cc-pwcVTZ-DK	0.985	1	D	0.999	1	R	0.959	1	R
M06-L/def2-TZVP	0.976	3	R	0.990	3	R	0.951	3	R
M06-L/def2-TZVPP	0.976	1	D	0.995	1	D	0.956	1	D
M06-L/ma-TZVP	0.977	1	R	0.991	1	R	0.952	1	R
M06-L/maug-cc-pVTZ	0.977	1	R	0.991	1	R	0.952	1	R
M06-L/MG3S	0.978	1	D	0.996	1	D	0.958	1	D
M08-HX/6-31+G(d,p)	0.972	1	D	0.983	1	D	0.944	1	D
M08-HX/aug-cc-pVTZ	0.975	1	R	0.989	1	R	0.950	1	R
M08-HX/cc-pVTZ+	0.974	1	D	0.985	1	D	0.946	1	D
M08-HX/def2-TZVPP	0.973	1	D	0.984	1	D	0.945	1	D
M08-HX/jun-cc-pVTZ	0.974	6	D	0.986	6	D	0.947	6	D
M08-HX/ma-TZVP	0.976	1	R	0.990	1	R	0.951	1	R
M08-HX/maug-cc-pVTZ	0.976	1	R	0.990	1	R	0.951	1	R
M08-HX/MG3S	0.973	1	D	0.984	1	D	0.946	1	D
M08-SO/6-31+G(d,p)	0.979	1	D	0.989	1	D	0.951	1	D
M08-SO/aug-cc-pVTZ	0.985	1	R	0.999	1	R	0.959	1	R
M08-SO/cc-pVTZ+	0.982	1	D	0.995	1	D	0.956	1	D
M08-SO/def2-TZVPP	0.980	1	D	0.993	1	D	0.954	1	D
M08-SO/ma-TZVP	0.984	1	R	0.998	1	R	0.958	1	R
M08-SO/maug-cc-pVTZ	0.983	1	R	0.997	1	R	0.957	1	R
M08-SO/MG3	0.984	4	D	0.998	4	R	0.959	4	R
M08-SO/MG3S	0.983	1	D	0.995	1	D	0.956	1	D
M08-SO/MG3SXP	0.984	1	D	0.996	1	D	0.957	1	D

M11-L/maug-cc-pVTZ	0.988	16	D	1.002	16	R	0.962	16	R
MN11-L/MG3S	0.985	16	D	0.999	16	R	0.959	16	R
MN12-L/jul-cc-pVDZ	0.974	14	R	0.988	14	R	0.950	14	R
MN12-L/MG3S	0.968	6	D	0.981	6	D	0.943	6	D
MN12-SX/6-311++G(d,p)	0.976	6	D	0.986	6	D	0.947	6	D
MN12-SX/jul-cc-pVDZ	0.979	14	R	0.993	14	R	0.954	14	R
MN15-L/MG3S	0.977	1	D	0.991	1	R	0.952	1	R
MN15-L/maug-cc-pVTZ	0.979	1	D	0.993	1	R	0.954	1	R
MC3BB	0.965	1	C	0.979	1	R	0.940	1	R
MC3MPW	0.964	1	C	0.977	1	R	0.939	1	R
MC-QCISD/3	0.992	1	C	1.006	1	R	0.966	1	R
MOHLYP/ma-TZVP	1.027	1	R	1.041	1	R	1.000	1	R
MOHLYP/MG3S	1.022	1	R	1.036	1	R	0.995	1	R
MP2(FC)/6-31+G(d,p)	0.968	1	C	0.982	1	R	0.943	1	R
MP2(FC)/6-311G(d,p)	0.970	1	R	0.984	1	R	0.945	1	R
MP2(FC)/6-31G(d)	0.964	1	R	0.977	1	R	0.939	1	R
MP2(FC)/6-31G(d,p)	0.958	1	R	0.971	1	R	0.933	1	R
MP2(FC)/cc-pVDZ	0.977	1	C	0.991	1	R	0.952	1	R
MP2(FC)/cc-pVTZ	0.975	1	D	0.992	1	D	0.953	1	D
MP2(FULL)/6-31G(d)	0.963	1	R	0.976	1	R	0.938	1	R
MP4(SDQ)/jul-cc-pVTZ	0.973	1	R	0.987	1	R	0.948	1	R
MPW1B95/6-31+G(d,p)	0.970	1	C	0.984	1	R	0.945	1	R
MPW1B95/MG3	0.970	1	C	0.984	1	R	0.945	1	R
MPW1B95/MG3S	0.972	1	C	0.986	1	R	0.947	1	R
MPW1K/6-31+G(d,p)	0.949	1	C	0.962	1	R	0.924	1	R
MPW1K/aug-cc-PDTZ	0.959	14	R	0.972	14	R	0.934	14	R
MPW1K/aug-cc-PVTZ	0.955	14	R	0.968	14	R	0.930	14	R
MPW1K/jul-cc-pVDZ	0.957	14	R	0.97	14	R	0.932	14	R
MPW1K/jul-cc-pVTZ	0.954	14	R	0.967	14	R	0.929	14	R
MPW1K/jun-cc-pVDZ	0.955	14	R	0.968	14	R	0.930	14	R
MPW1K/jun-cc-pVTZ	0.954	14	R	0.967	14	R	0.929	14	R
MPW1K/ma-TZVP	0.956	1	R	0.969	1	R	0.931	1	R
MPW1K/MG3	0.953	1	C	0.966	1	R	0.928	1	R
MPW1K/MG3S	0.956	1	C	0.969	1	R	0.931	1	R
MPW1K/MIDI!	0.953	1	R	0.966	1	R	0.928	1	R
MPW1K/MIDIY	0.947	1	R	0.960	1	R	0.922	1	R
MPW3LYP/6-31+G(d,p)	0.980	1	C	0.994	1	R	0.955	1	R
MPW3LYP/6-311+G(2d,p)	0.986	1	R	1.000	1	R	0.960	1	R
MPW3LYP/6-31G(d)	0.976	1	R	0.990	1	R	0.951	1	R
MPW3LYP/ma-TZVP	0.986	1	R	1.000	1	R	0.960	1	R
MPW3LYP/MG3S	0.982	1	C	0.996	1	R	0.956	1	R
MPW74/6-311+G(d,p)	0.912	2	C	0.888	2	R	0.925	2	R
MPW76/MG3S	0.909	2	C	0.885	2	R	0.922	2	R
MPWB1K/6-31+G(d,p)	0.951	1	C	0.964	1	R	0.926	1	R
MPWB1K/MG3S	0.954	1	C	0.967	1	R	0.929	1	R
MPWLYP1M/ma-TZVP	1.009	1	R	1.023	1	R	0.983	1	R

MW3.2//CCSD(T)-F12a/TZF	0.984	13	R	0.998	13	R	0.958	13	R
OreLYP/ma-TZVP	1.010	7	D	1.024	7	D	0.984	7	D
OreLYP/def2-TZVP	1.008	7	D	1.023	7	D	0.982	7	D
PBE/def2-TZVP	1.011	3	R	1.026	3	R	0.985	3	R
PBE/MG3S	1.010	1	D	1.025	1	D	0.985	1	D
PBE/ma-TZVP	1.014	1	D	1.028	1	D	0.987	1	D
PBE0/MG3S	0.975	1	D	0.989	1	D	0.950	1	D
PBE1KCIS/MG3	0.981	1	C	0.995	1	R	0.955	1	R
PBE1KCIS/MG3S	0.981	1	C	0.995	1	R	0.955	1	R
PM3	0.940	1	R	0.953	1	R	0.916	1	R
PM6	1.078	1	R	1.093	1	R	1.050	1	R
PW6B95/def2-TZVP	0.974	8	R	0.988	8	R	0.949	8	R
PWB6K/cc-pVDZ	0.953	12	D	0.966	12	R	0.928	12	R
QCISD/cc-pVTZ	0.975	11	R	0.989	11	R	0.950	11	R
QCISD/MG3S	0.978	10	R	0.992	10	R	0.953	10	R
QCISD(FC)/6-31G(d)	0.973	1	R	0.987	1	R	0.948	1	R
QCISD(T)/aug-cc-pVQZ	0.989	10	R	1.003	10	R	0.963	10	R
revTPSS/def2-TZVP	0.998	7	D	1.012	7	D	0.972	7	D
revTPSS/ma-TZVP	0.999	7	D	1.013	7	D	0.973	7	D
SOGGA/ma-TZVP	1.017	1	R	1.031	1	R	0.991	1	R
τHCTHhyb/ma-TZVP	0.989	1	R	1.003	1	R	0.963	1	R
TPSS1KCIS/def2-TZVP	0.982	1	R	0.996	1	R	0.956	1	R
TPSS1KCIS/ma-TZVP	0.983	1	R	0.997	1	R	0.957	1	R
TPSSh/MG3S	0.984	1	D	1.002	1	D	0.963	1	D
VSXC/MG3S	0.986	1	D	1.001	1	D	0.962	1	D
ωB97/def2-TZVP	0.969	1	R	0.983	1	R	0.944	1	R
ωB97/ma-TZVP	0.970	1	R	0.984	1	R	0.945	1	R
ωB97X/def2-TZVP	0.970	1	R	0.984	1	R	0.945	1	R
ωB97X/ma-TZVP	0.971	1	R	0.985	1	R	0.946	1	R
ωB97X-D/def2-TZVP	0.975	1	R	0.989	1	R	0.950	1	R
ωB97X-D/ma-TZVP	0.975	1	R	0.989	1	R	0.950	1	R
ωB97X-D/maug-cc-pVTZ	0.974	1	R	0.988	1	R	0.949	1	R
W3X//CCSD(T)-F12a/TZF	0.984	13	R	0.998	13	R	0.958	13	R
W3X-L//CCSD(T)-F12a/TZF	0.984	13	R	0.998	13	R	0.958	13	R
W3X-L//QCISD/STZ	0.973	13	R	0.987	13	R	0.948	13	R
X1B95/6-31+G(d,p)	0.968	1	C	0.982	1	R	0.943	1	R
X1B95/MG3S	0.971	1	C	0.985	1	R	0.946	1	R
XB1K/6-31+G(d,p)	0.952	1	C	0.965	1	R	0.927	1	R
XB1K/MG3S	0.955	1	C	0.968	1	R	0.930	1	R

References

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Methods

D: The scale factor was **d**irectly obtained from the ZPVE15/10 or F38/10 databases given in Ref. 1.
C: The scale factor was obtained by applying a small systematic **c**orrection of -0.0025 to preexisting scale factor. The references for the preexisting (uncorrected) scale factors are given in Supporting Information of Ref. 1 and in Version 1 of this database
R: The scale factor was obtained via the Reduced Scale Factor Optimization Model described in Ref. 1. Briefly, this entails using the ZPE6 database for determining ZPE scale factors, and/or using the universal scale factor ratios of $a^{F/ZPE} = 0.974$ and $a^{H/ZPE} = 1.014$ to obtain the respective values for the scale factors for fundamental and harmonic frequencies.