

Database of Frequency Scale Factors for Electronic Model Chemistries

—Version 5

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For thermochemistry and kinetics, use the ZPE scale factor.

For comparing with or predicting experimental IR spectra, use the F scale factor.

For comparing with harmonic frequencies from theory or experiment, use the H scale factor.

Methods:

D: The scale factor was directly obtained from the ZPVE15/10 or F38/10 databases given in Ref. 1.

C: The scale factor was obtained by applying a small systematic correction of -0.0025 to a 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 $\alpha^{F/ZPE} = 0.974$ and $\alpha^{H/ZPE} = 1.014$ to obtain the respective values for the scale factors for fundamental and harmonic frequencies.

Model Chemistry	Scale factor						
	Ref.	Zero Point Energy (ZPE)		Harmonic Frequencies (H)		Fundamentals (F)	
		Value	Method	Value	Method	Value	Method
AM1	1	0.948	R	0.961	R	0.923	R
B1B95/6-31+G(d,p)	1	0.971	C	0.985	R	0.946	R
B1B95/MG3S	1	0.973	C	0.987	R	0.948	R
B1LYP/MG3S	1	0.978	D	0.994	D	0.955	D
B3LYP/6-31G(2df,2p)	1	0.981	C	0.995	R	0.955	R
B3LYP/6-31G(d)	1	0.977	R	0.991	R	0.952	R
B3LYP/6-311++G(d,p)	27	0.985	D	0.998	R	0.959	R
B3LYP/aug-cc-pVTZ	3	0.985	R	0.999	R	0.959	R
B3LYP/def2-TZVP	3	0.985	R	0.999	R	0.959	R
B3LYP/ma-TZVP	1	0.986	R	1.000	R	0.960	R
B3LYP/MG3S	1	0.983	D	0.998	D	0.960	D
B3P86/6-31G(d)	1	0.971	R	0.985	R	0.946	R
B3PW91/6-31G(d)	1	0.972	R	0.986	R	0.947	R
B97-3/def2-TZVP	8	0.974	D	0.988	R	0.949	R
B97-3/ma-TZVP	1	0.975	R	0.989	R	0.950	R
B97-3/MG3S	1	0.972	D	0.986	D	0.947	D
B98/def2-TZVP	1	0.984	R	0.998	R	0.958	R
B98/ma-TZVP	1	0.985	R	0.999	R	0.959	R
B98/MG3S	1	0.982	D	0.995	D	0.956	D
BB1K/6-31+G(d,p)	1	0.954	C	0.967	R	0.929	R
BB1K/MG3S	1	0.957	C	0.970	R	0.932	R
BB95/6-31+G(d,p)	1	1.011	C	1.025	R	0.985	R
BB95/MG3S	1	1.012	C	1.026	R	0.986	R

Model Chemistry	Scale factor						
	Ref.	Zero Point Energy (ZPE)		Harmonic Frequencies (H)		Fundamentals (F)	
		Value	Method	Value	Method	Value	Method
BLYP/6-31G(d)	1	1.009	R	1.023	R	0.983	R
BLYP/6-311G(df,p)	1	1.013	R	1.027	R	0.987	R
BLYP/MG3S	27	1.013	D	1.027	R	0.987	R
BMC-CCSD	1	0.985	D	1.001	D	0.962	D
BMK/ma-TZVP	1	0.972	R	0.986	R	0.947	R
BMK/MG3S	1	0.971	D	0.984	D	0.945	D
BP86/6-31G(d)	1	1.007	R	1.021	R	0.981	R
BP86/ma-TZVP	1	1.014	R	1.028	R	0.988	R
BPW60/6-311+G(d,p)	2	0.934	C	0.947	R	0.910	R
BPW63/MG3S	2	0.923	C	0.936	R	0.899	R
CAM-B3LYP/ma-TZVP	1	0.976	R	0.990	R	0.951	R
CASPT2(11,9)/aug-cc-pVTZ	20	0.957	D	0.970	R	0.932	R
CCSD/jul-cc-pVTZ	1	0.973	R	0.987	R	0.948	R
CCSD-F12/jul-cc-pVTZ	1	0.971	R	0.985	R	0.946	R
CCSD(T)/aug-cc-pVTZ	1	0.987	R	1.001	R	0.961	R
CCSD(T)/jul-cc-pVTZ	1	0.984	R	0.998	R	0.958	R
CCSD(T)-F12/jul-cc-pVTZ	1	0.981	R	0.995	R	0.955	R
CCSD(T)-F12a/cc-pVDZ-F12	11	0.983	R	0.997	R	0.957	R
CCSD(T)-F12a/cc-pVTZ-F12	1	0.984	R	0.998	R	0.958	R
CCSD(T)-F12a/jun-cc-pVTZ	20	0.984	D	0.998	R	0.958	R
CCSD(T)-F12a/TZF	13	0.984	R	0.998	R	0.958	R
DCSD-F12a/cc-pVDZ-F12	30	0.967	D	0.981	R	0.942	R
DF-CCSD(T)-F12b/cc-pVDZ-F12	30	0.983	D	0.997	R	0.957	R
DF-CCSD(T)-F12b/jun-cc-pVDZ-F12	30	0.981	D	0.995	R	0.955	R
G96LYP80/6-311+G(d,p)	2	0.911	C	0.924	R	0.887	R
G96LYP82/MG3S	2	0.907	C	0.920	R	0.883	R
GAM/def2-TZVP	7	0.980	D	0.994	D	0.955	D
GAM/ma-TZVP	7	0.981	D	0.995	D	0.956	D
HF/3-21G	1	0.919	R	0.932	R	0.895	R
HF/6-31+G(d)	1	0.911	R	0.924	R	0.887	R
HF/6-31+G(d,p)	1	0.915	C	0.928	R	0.891	R
HF/6-311G(d,p)	1	0.920	R	0.933	R	0.896	R
HF/6-311G(df,p)	1	0.920	R	0.933	R	0.896	R
HF/6-31G(d)	1	0.909	R	0.922	R	0.885	R
HF/6-31G(d,p)	1	0.913	R	0.926	R	0.889	R
HF/MG3S	1	0.919	D	0.932	D	0.895	D
HFLYP/MG3S	1	0.899	D	0.912	D	0.876	D
HSEh1PBE/ma-TZVP	1	0.979	R	0.993	R	0.954	R
M05/aug-cc-pVTZ	1	0.978	R	0.992	R	0.953	R
M05/def2-TZVP	3	0.978	R	0.991	R	0.952	R
M05/ma-TZVP	1	0.979	R	0.993	R	0.954	R
M05/maug-cc-pVTZ	1	0.978	R	0.992	R	0.953	R

Model Chemistry	Scale factor						
	Ref.	Zero Point Energy (ZPE)		Harmonic Frequencies (H)		Fundamentals (F)	
		Value	Method	Value	Method	Value	Method
M05/MG3S	1	0.977	D	0.989	D	0.951	D
M05-2X/6-31+G(d,p)	1	0.961	D	0.974	D	0.936	D
M05-2X/aug-cc-pVTZ	1	0.964	R	0.977	R	0.939	R
M05-2X/def2-TZVPP	1	0.962	D	0.976	D	0.938	D
M05-2X/ma-TZVP	1	0.965	R	0.979	R	0.940	R
M05-2X/maug-cc-pVTZ	1	0.964	R	0.977	R	0.939	R
M05-2X/MG3S	1	0.962	D	0.975	D	0.937	D
M06/6-31+G(d,p)	27	0.980	D	0.994	D	0.955	D
M06/6-311+G(d,p)	27	0.983	D	0.997	R	0.957	R
M06/aug-cc-pVTZ	1	0.984	R	0.998	R	0.958	R
M06/def2-TZVP	3	0.982	R	0.996	R	0.956	R
M06/def2-TZVPP	1	0.979	D	0.992	D	0.953	D
M06/def2-SVP	18	0.982	D	0.996	D	0.957	D
M06/ma-TZVP	1	0.982	R	0.996	R	0.956	R
M06/maug-cc-pVTZ	1	0.982	R	0.996	R	0.956	R
M06/MG3S	1	0.981	D	0.994	D	0.955	D
M06-2X/6-31G(d,p)	28	0.965	D	0.979	R	0.940	R
M06-2X/6-31+G(d,p) ^a	27	0.968	D	0.981	D	0.942	D
M06-2X/6-311G(d,p) ^a	27	0.968	D	0.982	R	0.943	R
M06-2X/6-311+G(d,p)	5	0.970	D	0.983	R	0.944	R
M06-2X/6-311++G(d,p)	5	0.970	D	0.983	R	0.944	R
M06-2X/aug-cc-pVDZ	14	0.979	D	0.993	R	0.954	R
M06-2X/aug-cc-pVTZ	1	0.971	D	0.985	D	0.946	D
M06-2X/def2-QZVP	7	0.970	D	0.983	D	0.945	D
M06-2X/def2-TZVP	7	0.971	D	0.984	D	0.946	D
M06-2X/def2-TZVPP	1	0.970	D	0.983	D	0.945	D
M06-2X/jul-cc-pVDZ	14	0.977	D	0.991	R	0.952	R
M06-2X/jul-cc-pVTZ	14	0.971	D	0.985	R	0.946	R
M06-2X/jun-cc-pVDZ	14	0.976	D	0.990	R	0.951	R
M06-2X/jun-cc-pVTZ	14	0.971	D	0.985	R	0.946	R
M06-2X/ma-TZVP	1	0.972	R	0.986	R	0.947	R
M06-2X/maug-cc-pV(T+d)Z	1	0.971	D	0.984	D	0.945	D
M06-2X/may-cc-pVTZ	24	0.971	D	0.985	R	0.946	R
M06-2X/MG3S	1	0.970	D	0.983	D	0.944	D
M06CR/MG3S	30	0.980	D	0.994	R	0.955	R
M06-HF/6-31+G(d,p)	1	0.954	D	0.969	D	0.931	D
M06-HF/aug-cc-pVTZ	1	0.961	R	0.974	R	0.936	R
M06-HF/def2-TZVPP	1	0.958	D	0.970	D	0.932	D
M06-HF/ma-TZVP	1	0.957	R	0.970	R	0.932	R
M06-HF/maug-cc-pVTZ	1	0.959	R	0.972	R	0.934	R
M06-HF/MG3S	1	0.955	D	0.967	D	0.930	D
M06-L/6-31G(d)	26	0.976	D	0.991	D	0.951	D
M06-L/6-31G(d,p)	15	0.977	D	0.991	R	0.952	R
M06-L/6-31+G(d,p)	1	0.978	D	0.992	D	0.953	D

Model Chemistry	Scale factor						
	Ref.	Zero Point Energy (ZPE)		Harmonic Frequencies (H)		Fundamentals (F)	
		Value	Method	Value	Method	Value	Method
M06-L/aug-cc-pVTZ	1	0.980	R	0.994	R	0.955	R
M06-L/aug-cc-pV(T+d)Z	9	0.980	R	0.994	R	0.955	R
M06-L/aug-cc-pVTZ-pp	9	0.980	R	0.994	R	0.955	R
M06-L/def2-TZVP	3	0.976	R	0.990	R	0.951	R
M06-L/def2-TZVPP	27	0.976	D	0.990	D	0.951	D
M06-L/ma-TZVP	1	0.977	R	0.991	R	0.952	R
M06-L/maug-cc-pVTZ	1	0.977	R	0.991	R	0.952	R
M06-L/MG3S	27	0.978	D	0.992	D	0.952	D
M06-L(DKH2)/aug-cc-pwcVTZ-DK	1	0.985	D	0.999	R	0.959	R
M08-HX/6-31+G(d,p)	27	0.972	D	0.986	R	0.947	R
M08-HX/aug-cc-pVTZ	1	0.975	R	0.989	R	0.950	R
M08-HX/cc-pVTZ+	27	0.974	D	0.988	R	0.949	R
M08-HX/def2-TZVPP	27	0.973	D	0.987	R	0.948	R
M08-HX/jun-cc-pVTZ	27	0.974	D	0.988	R	0.949	R
M08-HX/ma-TZVP	1	0.976	R	0.990	R	0.951	R
M08-HX/maug-cc-pVTZ	1	0.976	R	0.990	R	0.951	R
M08-HX/may-cc-pVTZ	25	0.974	D	0.988	R	0.949	R
M08-HX/MG3S	27	0.973	D	0.986	R	0.948	R
M08-SO/6-31+G(d,p)	27	0.979	D	0.993	R	0.954	R
M08-SO/aug-cc-pVTZ	1	0.985	R	0.999	R	0.959	R
M08-SO/cc-pVTZ+	1	0.982	D	0.995	D	0.956	D
M08-SO/def2-TZVPP	1	0.980	D	0.993	D	0.954	D
M08-SO/jun-cc-pVTZ	19	0.984	D	0.998	D	0.958	R
M08-SO/ma-TZVP	1	0.984	R	0.998	R	0.958	R
M08-SO/maug-cc-pVTZ	1	0.983	R	0.997	R	0.957	R
M08-SO/MG3	4	0.984	D	0.998	R	0.959	R
M08-SO/MG3S	1	0.983	D	0.995	D	0.956	D
M08-SO/MG3SXP	1	0.984	D	0.996	D	0.957	D
M11-L/maug-cc-pVTZ	16	0.988	D	1.002	R	0.962	R
M11-L/MG3S	16	0.985	D	0.999	R	0.959	R
MN12-L/jul-cc-pVDZ	14	0.974	R	0.988	R	0.950	R
MN12-L/MG3S	6	0.968	D	0.981	D	0.943	D
MN12-SX/6-311++G(d,p)	27	0.976	D	0.989	D	0.950	D
MN12-SX/jul-cc-pVDZ	14	0.979	R	0.993	R	0.954	R
MN15/aug-cc-pVTZ	17	0.976	D	0.990	D	0.950	D
MN15/def2-SVP	18	0.973	D	0.986	D	0.947	D
MN15/ma-TZVP	17	0.975	D	0.989	D	0.950	D
MN15-L/def2-TZVP	29	0.980	D	0.994	R	0.955	R
MN15-L/maug-cc-pVTZ	1	0.979	D	0.993	R	0.954	R
MN15-L/MG3S	21	0.973	D	0.987	R	0.947	R
MC3BB	1	0.965	C	0.979	R	0.940	R
MC3MPW	1	0.964	C	0.977	R	0.939	R
MC-QCISD/3	1	0.992	C	1.006	R	0.966	R
MOHLYP/ma-TZVP	1	1.027	R	1.041	R	1.000	R

Model Chemistry	Scale factor						
	Ref.	Zero Point Energy (ZPE)		Harmonic Frequencies (H)		Fundamentals (F)	
		Value	Method	Value	Method	Value	Method
MOHLYP/MG3S	1	1.022	R	1.036	R	0.995	R
MP2(FC)/6-31G(d)	1	0.964	R	0.977	R	0.939	R
MP2(FC)/6-31G(d,p)	1	0.958	R	0.971	R	0.933	R
MP2(FC)/6-31+G(d,p)	1	0.968	C	0.982	R	0.943	R
MP2(FC)/6-311G(d,p)	1	0.970	R	0.984	R	0.945	R
MP2(FC)/cc-pVDZ	1	0.977	C	0.991	R	0.952	R
MP2(FC)/cc-pVTZ	27	0.975	D	0.989	R	0.950	R
MP2(FULL)/6-31G(d)	1	0.963	R	0.976	R	0.938	R
MP4(SDQ)/jul-cc-pVTZ	1	0.973	R	0.987	R	0.948	R
MPW1B95/6-31+G(d,p)	1	0.970	C	0.984	R	0.945	R
MPW1B95/MG3	1	0.970	C	0.984	R	0.945	R
MPW1B95/MG3S	1	0.972	C	0.986	R	0.947	R
MPW1K/6-31+G(d,p)	1	0.949	C	0.962	R	0.924	R
MPW1K/aug-cc-PDTZ	14	0.959	R	0.972	R	0.934	R
MPW1K/aug-cc-PVTZ	14	0.955	R	0.968	R	0.930	R
MPW1K/jul-cc-pVDZ	14	0.957	R	0.970	R	0.932	R
MPW1K/jul-cc-pVTZ	14	0.954	R	0.967	R	0.929	R
MPW1K/jun-cc-pVDZ	14	0.955	R	0.968	R	0.930	R
MPW1K/jun-cc-pVTZ	14	0.954	R	0.967	R	0.929	R
MPW1K/ma-TZVP	1	0.956	R	0.969	R	0.931	R
MPW1K/MG3	1	0.953	C	0.966	R	0.928	R
MPW1K/MG3S	1	0.956	C	0.969	R	0.931	R
MPW1K/MIDI! \equiv MPW1K/MIDIX	1	0.953	R	0.966	R	0.928	R
MPW1K/MIDIY	1	0.947	R	0.960	R	0.922	R
MPW3LYP/6-31G(d)	1	0.976	R	0.990	R	0.951	R
MPW3LYP/6-31+G(d,p)	1	0.980	C	0.994	R	0.955	R
MPW3LYP/6-311+G(2d,p)	1	0.986	R	1.000	R	0.960	R
MPW3LYP/ma-TZVP	1	0.986	R	1.000	R	0.960	R
MPW3LYP/MG3S	1	0.982	C	0.996	R	0.956	R
MPW74/6-311+G(d,p)	2	0.912	C	0.925	R	0.888	R
MPW76/MG3S	2	0.909	C	0.922	R	0.885	R
MPWB1K/6-31+G(d,p)	1	0.951	C	0.964	R	0.926	R
MPWB1K/MG3S	1	0.954	C	0.967	R	0.929	R
MPWLYP1M/ma-TZVP	1	1.009	R	1.023	R	0.983	R
OreLYP/ma-TZVP	7	1.010	D	1.024	D	0.984	D
OreLYP/def2-TZVP	7	1.008	D	1.023	D	0.982	D
PBE/6-31G** \equiv PBE/6-31G(d,p)	17	1.006	D	1.020	D	0.980	D
PBE/aug-cc-pVTZ	17	1.012	D	1.027	D	0.986	D
PBE/def2-TZVP	3	1.011	R	1.026	R	0.985	R
PBE/ma-TZVP	1	1.014	D	1.028	D	0.987	D
PBE/MG3S	1	1.010	D	1.025	D	0.985	D
PBE0/MG3S	1	0.975	D	0.989	D	0.950	D
PBE1KCIS/MG3	1	0.981	C	0.995	R	0.955	R

Model Chemistry	Scale factor						
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PBE1KCIS/MG3S	1	0.981	C	0.995	R	0.955	R
PM3	1	0.940	R	0.953	R	0.916	R
PM6	1	1.078	R	1.093	R	1.050	R
PM7	22	1.078	D	1.093	R	1.050	R
PW6B95/def2-TZVP	8	0.974	R	0.988	R	0.949	R
PWB6K/cc-pVDZ	12	0.953	D	0.966	R	0.928	R
QCISD/cc-pVTZ	11	0.975	R	0.989	R	0.950	R
QCISD/MG3S	10	0.978	R	0.992	R	0.953	R
QCISD/6-311++G(2df,2p)	13	0.973	R	0.987	R	0.948	R
QCISD(FC)/6-31G(d)	1	0.973	R	0.987	R	0.948	R
QCISD(T)/aug-cc-pVQZ	10	0.989	R	1.003	R	0.963	R
revM06/ma-TZVP	17	0.970	D	0.984	D	0.945	D
revM06/MG3S	23	0.968	D	0.981	R	0.943	R
revM06-L/def2-TZVP	29	0.972	D	0.986	R	0.947	R
revTPSS/def2-TZVP	7	0.998	D	1.012	D	0.972	D
revTPSS/ma-TZVP	7	0.999	D	1.013	D	0.973	D
SOGGA/ma-TZVP	1	1.017	R	1.031	R	0.991	R
τ HCTHhyb/ma-TZVP	1	0.989	R	1.003	R	0.963	R
TPSS1KCIS/def2-TZVP	1	0.982	R	0.996	R	0.956	R
TPSS1KCIS/ma-TZVP	1	0.983	R	0.997	R	0.957	R
TPSSh/MG3S	1	0.984	D	0.998	R	0.958	R
VSXC/MG3S	1	0.986	D	1.001	D	0.962	D
ω B97/def2-TZVP	1	0.969	R	0.983	R	0.944	R
ω B97/ma-TZVP	1	0.970	R	0.984	R	0.945	R
ω B97X/def2-TZVP	1	0.970	R	0.984	R	0.945	R
ω B97X/ma-TZVP	1	0.971	R	0.985	R	0.946	R
ω B97X-D/6-31G (d,p)	27	0.968	D	0.982	R	0.943	R
ω B97X-D/6-31+G (d,p)	27	0.971	D	0.985	R	0.946	R
ω B97X-D/def2-TZVP	1	0.975	R	0.989	R	0.950	R
ω B97X-D/ma-TZVP	1	0.975	R	0.989	R	0.950	R
ω B97X-D/maug-cc-pVTZ	1	0.974	R	0.988	R	0.949	R
X1B95/6-31+G (d,p)	1	0.968	C	0.982	R	0.943	R
X1B95/MG3S	1	0.971	C	0.985	R	0.946	R
XB1K/6-31+G (d,p)	1	0.952	C	0.965	R	0.927	R
XB1K/MG3S	1	0.955	C	0.968	R	0.930	R

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