

List of Abbreviations

<i>Abbreviation</i>	<i>Full form</i>
AIMD	Ab-initio Molecular Dynamics
B3LYP	Becke, 3-parameter, Lee-Yang-Parr
BO	Born-Oppenheimer
BOA	Born-Oppenheimer Approximation
BOMD	Born-Oppenheimer Molecular Dynamics
CC	Coupled Cluster
c-C ₃ H ₄ O ₂	3-oxetanone
CCSD(T)	Coupled Cluster Single Double (Triple)
CF ₂ Br ₂	Dichlorodibromomethane (Halon 1202)
CF ₂ Cl ₂	Dichlorodifluoromethane (Freon-12)
CFCs	Chlorofluorocarbons
CH ₂ BrCl	Bromochloromethane
CH ₂ CO	Ketene
CH ₃ C(O)N ₃	Acetyl azide
CHBr ₃	Bromoform
CI	Configuration Interaction
CO	Carbon monoxide
CP	Car Parrinello
DFT	Density Functional Theory
ESCs	Electronic Structure Calculations
FC(O)N ₃	Fluorocarbonyl azide
Halons	Halomethanes
IRC	Intrinsic Reaction Coordinate
IVR	Intramolecular Vibrational energy Redistribution
K.E.	Kinetic Energy
LEPS	London-Eyring-Polanyi-Sato
MAD	Mean absolute deviation
MD	Molecular Dynamics
MM	Molecular Mechanics
MP2	Second-order Moller-Plesset Perturbation
NWChem	NorthWest Computational Chemistry
P.E.	Potential Energy
PBE	Perdew-Burke-Ernzerhof (PBE)
PES	Potential Energy Surface
QM	Quantum Mechanics
RRKM	Rice-Ramsperger-Kassel-Marcus
TS	Transition State
ZPE	Zero Point Energy

