Important List of Abbreviations

AIM  Atoms in molecules
AO   Atomic Orbital
B3LYP Becke 3 Lee Yang Parr
BSSE Basis Set Superposition Error
CI   Configuration Interaction
CP   Counterpoise
DFT  Density Functional Theory
GTO  Gaussian Type Orbital
GS   Ground State
GTF  Gaussian Type Function
HF   Hartree Fock Energy
L1   Theoretical Level B3LYP/6-31+G*
L2   Theoretical Level B3LYP/Aug-cc-pVDZ
L3   Theoretical Level MP2/6-31+G*
L4   Theoretical Level MP2/ Aug-cc-pVDZ
MO   Molecular Orbital
MP2  Moller-Plesset Second Order
NBO  Natural Bond Orbital
NPA  Natural Population Analysis
PA   Proton Affinity
PCM  Polarized Continuum Model
PES  Potential Energy Surface
RHF  Restricted Hartree Fock
RTS  Rotational Transition State
SCF  Self Consistent Field
STO  Slater Type Orbital
TS   Transition State
UHF  Unrestricted Hartree Fock
ZPVE Zero point Vibrational Energy
CBS  Complete basis set