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LIST OF ABBREVIATIONS

AM1	=	Austin Model 1
au	=	atomic units
B3LYP	=	Becke's three parameter hybrid functional using the LYP correlation functional
BSSE	=	basis set superposition error
C_h	=	chiral vector
CNT	=	Carbon nanotube
CP	=	counterpoise method
DFT	=	density functional theory
eV	=	electron volt
FMO	=	Frontier Molecular Orbital
FTIR	=	Fourier transform infrared spectroscopy
HOMO	=	Highest Occupied Molecular Orbital
IR	=	infrared spectroscopy
kcal	=	kilocalories
LUMO	=	Lowest Unoccupied Molecular Orbital
LYP	=	Lee-Yang-Parr functional
MO	=	molecular orbital
MWNT	=	Multi-walled carbon nanotube
η	=	Chemical hardness
ONIOM	=	our Own N-layered Integrated molecular Orbital and molecular Mechanics
pm	=	picometer
PBE	=	Perdew-Burke-Ernzerhof functional
QM	=	quantum mechanics
SCF	=	self-consistent field
SWNT	=	Single-walled carbon nanotube
ZPE	=	zero-point energy