

Abbreviations

B3LYP	Becke-3 parameter density functional theory with Lee–Yang–Parr correlation functional
BP	Becke and Perdew–Wang functionals
CIDNP	Chemically induced dynamic nuclear polarization
CP/MAS	Cross polarization/magic angle spinning
DF	Density functional
DFT	Density functional theory
DMF	Dimethylformamide
DMSO	Dimethylsulfoxide
EC	Electrochemical (oxidation, reduction)
ENDOR	Electron-nuclear double resonance
EPR	Electron paramagnetic resonance
ESR	Electron spin resonance
FTIR	Fourier transformation infrared (spectroscopy)
HEDM	High energy density materials
HFS	Hyperfine structure
HOMO	Highest occupied molecular orbital
HPLC	High-performance liquid chromatography
HTS	High-throughput screening
IR	Infrared
LUMO	Lowest unoccupied molecular orbital
METRO	Metronidazole
MP2	Moller–Plesset second-order perturbation method
NMR	Nuclear magnetic resonance
NOE	Nuclear Overhauser effect
NQR	Nuclear quadruple resonance
NTO	3-Nitro-1,2,4-triazole-5-one
PE	Photoelectron spectra
pK_a	Acidity constant
pK_{BH^+}	Basicity constant
PM3	Parametrized model 3
PWC	Perdew–Wang functional

QSAR	Quantitative structure-activity relationship
RA	Radical anion
RDA	Radical dianion
RDER	Rotating disk electrode with a ring
SOPPA	Secondary order polarization propagator approximation
TNBN	2,4,6-Trinitrobenzonitrile
TNT	2,4,6-Trinitrotoluene
UHF	Unrestricted Hartree Fock
UV	Ultraviolet
VNS	Vicarious nucleophilic substitution

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