

Abbreviations

%N	percentage nitrogen by mass
2-NDPA	2-Nitrodiphenylamine
AIMD	<i>ab initio</i> molecular dynamics
AO	atomic orbital
a.u.	atomic units
B3LYP	Becke, 3-parameter, Lee-Yang-Parr hybrid functional
BCP	bonding critical point
BSSE	basis set superposition error
CH₃CH₃	NC repeat unit with two –OCH ₃ capping groups
CH₃OH	NC repeat unit with –OCH ₃ capping group on ring 1 and –OH group on ring 2
CCP	cage critical point
CP	critical point
DFT	density functional theory
DFT-D	density functional theory with dispersion correction
DSC	differential scanning calorimetry
DOS	degree of substitution
DPA	diphenylamine

EM	energetic materials
EN	ethyl nitrate
ESP	electrostatic potential
G09	Gaussian 09 revision D.01
GGA	generalised gradient approximation
GM	genetically modified
GTO	Gaussian type orbitals
GView	Gauss View 5.0.8
HF	Hartree-Fock
HMF	hydroxymethylfurfural
HOMO	highest occupied molecular orbital
IR	infra-red spectroscopy
KS-DFT	Kohn-Sham DFT
LDA	local density approximation
MD	molecular dynamics
MEP	minimum energy path
MM	molecular mechanics
MMFF94	Merck molecular force field 94
MO	molecular orbitals
MP2	Møller–Plesset perturbation theory with second order correction
MW	molecular weight
NBO	natural bond orbital
NC	nitrocellulose

NCP	nuclear critical point
NG	nitroglycerine
NMR	nuclear magnetic resonance spectroscopy
OHCH₃	NC repeat unit with –OH capping group on ring 1 and –OCH ₃ group on ring 2
PCM	polarisable continuum model
PES	potential energy surface
PETN	pentaerythritol tetranitrate
PETRIN	pentaerythritol trinitrate
QM	quantum mechanics
QTAIM	quantum theory of atoms in molecules
RCP	ring critical point
RESP	restrained electrostatic potential atomic partial charges
RHF	restricted HF
ROHF	restricted-open HF
UHF	unrestricted HF
SB59	1,4-bis(ethylamino)-9,10-anthraquinone dye
SCF	self-consistent field
SEM	scanning electron microscopy
SMD	solvation model based on density
S_N2	bi-molecular nucleophilic substitution reaction
STO	Slater type orbitals
TG	thermogravimetric analysis

TS	transition state
UFF	universal force field
UV	ultraviolet
UVvis	ultraviolet–visible spectroscopy
vdW	van der Waals
ωB97X-D	ω B97X-D long-range corrected hybrid functional
ZPE	zero-point energy