

# Abbreviations

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

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

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

<b>TS</b>	transition state
<b>UFF</b>	universal force field
<b>UV</b>	ultraviolet
<b>UVvis</b>	ultraviolet–visible spectroscopy
<b>vdW</b>	van der Waals
<b><math>\omega</math>B97X-D</b>	$\omega$ B97X-D long-range corrected hybrid functional
<b>ZPE</b>	zero-point energy