

LIST OF ABBREVIATIONS

5-ASA	:	5-aminosalicylic acid
asyd	:	asymmetric deformation
asydo	:	out of plane asymmetric deformation
asyt	:	asymmetric torsion
asyto	:	out of plane asymmetric torsion
B3	:	Becke-3parameter exchange functional
B3LYP	:	Becke-3-Lee-Yang-Parr
BLYP	:	Becke-Lee-Yang-Parr
CCD	:	Charged coupled device
CDNBA	:	4-chloro-3, 5-dinitrobenzoic acid
DFT	:	Density functional theory
DLATGS	:	deuterated l-alanine-doped triglycine sulfate
EC	:	Ethyl centralite
ED	:	Electron density
FMO	:	Frontier molecular orbital
FT	:	Fourier transform
FTIR	:	Fourier transform infrared
Ge	:	Germanium
GTO	:	Gaussian type orbitals
HDL-C	:	High-density lipoprotein cholesterol
HF	:	Hartree-Fock
HOMA	:	Harmonic oscillator model of aromaticity
HOMO	:	Highest occupied molecular orbital
H-NMR	:	Hydrogen-nuclear magnetic resonance
IBD	:	Inflammatory bowel disease
ICT	:	Intramolecular charge transfer
ipb	:	in plane bending
ipr	:	in plane rocking
ips	:	in plane stretching

IR	:	Infrared
KBr	:	Potassium bromide
LCAO	:	Linear combination of atomic orbitals
LUMO	:	Lowest unoccupied molecular orbital
LYP	:	Lee-Yang-Parr correlation functional
MCT	:	mercury cadmium telluride
Me	:	Methyl
Mn	:	Methylene
MO	:	Molecular orbitals
N ₂	:	Nitrogen
NaCl	:	Sodium chloride
NBO	:	Natural bond orbital
NCA	:	Normal coordinate analysis
Nd:YAG	:	Neodimium: Yttrium-aluminium-garnet
NLO	:	Nonlinear optical
opb	:	out of plane bending
opr	:	out of plane rocking
ops	:	out of plane stretching
PED	:	Potential energy distribution
Ph	:	Phenyl
PNMC	:	3-methyl-4-nitrophenol
PNOC	:	2-methyl-4-nitrophenol
puck	:	puckering
Py	:	Pyridine
Pym	:	Pyrimidine
QTH	:	quartz-tungsten-halogen
RMS	:	Root mean square
roc	:	rocking
SCF	:	Self-consistent field
sci	:	scissoring
ss	:	symmetric stretching
STO	:	Slater type orbitals

STO-3G	:	Slater type orbital three Gaussians
SQM	:	Scaled quantum mechanical
SQMFF	:	Scaled quantum mechanical force field
TD-DFT	:	Time dependent density functional theory
trid	:	trigonal deformation
twi	:	twisting
UV	:	Ultraviolet
UV-vis	:	Ultraviolet-visible
wag	:	wagging
XRD	:	X-ray diffraction

LIST OF SYMBOLS USED

α	:	linear polarizability
β	:	first order hyperpolarizability
δ	:	in-plane bending
η	:	Electron localization function
μ	:	dipole moment
ν	:	stretching
τ	:	torsion
ω	:	wagging