

LIST OF ABBREVIATIONS

Abbreviation	Name
B3LYP	- Becke3-Lee-Yang-Parr
COOP	- Crystal orbital overlap population
CVT	- Chemical Vapour Transport
DFT	- Density functional theory
DOS	- Density of states
FT	- Fourier Transform
FT-IR	- Fourier Transform Infrared
HF	- Hartree-Fock
HOMO	- Highest occupied molecular orbital
ICT	- Intramolecular charge transfer
IR	- Infrared
KDP	- Potassium dihydrogen phosphate
LLS	- L-Leucinium squarate monohydrate
LUMO	- Lowest unoccupied molecular orbital
MEP	- Molecular electrostatic potential
NAO	- Natural Orbital Analysis
NBO	- Natural bond orbital
NLO	- Non-linear optics

PDNB	- Potassium 3,5-Dinitrobenzoate
PDOS	- Partial density of states
PED	- Potential energy distribution
PES	- Potential energy surface
PVT	- Physical Vapour Transport
PVT	- Physical vapour transport
PXRD	- Powder X-ray Diffractometer
SHG	- Second Harmonic Generation
SXRD	- Single Crystal X-ray Diffractometer
TD-DFT	- Time dependent density function theory
TONP	- Triphenylphosphine oxide 4- nitrophenol
TPPO	- Triphenylphosphine oxide
UV-vis	- Ultraviolet
XRD	- X-ray diffraction
ZNB	- Zinc Benzoate
ZSD	- Zinc Salicilate

LIST OF SYMBOLS

Symbol	Name
α	Linear Polarization
β	First-order hyperpolarizability
γ	Second-order hyperpolarizability
\AA	Armstrong
ν_{as}	asymmetric stretching
ν_s	symmetric stretching
δ	scissoring
ρ	rocking
τ	torsion