LIST OF ABBREVIATIONS

$T$  
Kinetic energy

$2$CP  
2-cyanopyridine

$2$FP  
2-fluoropyridine

$2$MIC  
2-Methoxyphenyl isocyanate

$2$MIT  
2-Methoxyphenyl isothiocyanate

$3$CPF  
3-cyano-2-fluoropyridine

$3$CP  
3-cyanopyridine

$3$FP  
3-fluoropyridine

$3$MPI  
(R)-(+)1-(3-Methoxyphenyl)ethyl isocyanate

$4$-BrNCO  
(R)-(+)1-(4-Bromophenyl) ethyl isocyanate

$4$-BrNCS  
(R)-(+)1-(4-Bromophenyl) ethyl isothiocyanate

$4$CP  
4-cyanopyridine

$4$FP  
4-fluoropyridine

$4$FPI  
(R)-(+)1-(4- Fluorophenyl) ethyl isocyanate

$4$MPI  
(R)-(+)1-(4-Methoxyphenyl)ethyl isocyanate

Å$^4$/amu  
Fourth power of angstrom per atomic mass unit

amuÅ$^2$  
atomic mass unit per angstrom square

B3LYP  
Becke’s Lee Yang Parr

BD  
Bond orbital

BD*  
Anti-bonding orbital

BSSE  
Basis set superposition error

D  
debyes

DFT  
Density functional theory

EDTM  
Electric dipole transition moment

Expt  
Experimental
FT  Fourier transform
h  hartree
HOMO  Highest occupied molecular orbital
hu  hump
LP  Lone pair
LUMO  Lowest unoccupied molecular orbital
MAD  Mean absolute deviation
MDTM  Magnetic dipole transition moment
MHz  megahertz
NBO  Natural bond orbital
PED  Potential energy distribution
PEM  photo elastic modulator
PES  Potential energy surface
PIC  Phenyl isocyanate
PIT  Phenyl isothiocyanate
R  Rotational strength
RHF  Restricted Hartree Fock
RMS  Root mean square
ROA  Raman optical activity
sh  shoulder
V  Potential energy
VCD  Vibrational circular dichroism
VOA  Vibrational optical activity
XRD  X-ray diffraction
μ  Dipole moment
μ  Reduced mass
v  Frequency