### List of Figures

| Figure 1.1 | Schematic diagram of Michelson interferometer | 4  |
| Figure 1.2 | Layout of Brucker IFS 66V Fourier transform spectrometer | 5  |
| Figure 1.3 | Polarisation (P) induced in a molecule’s electron cloud | 8  |
| Figure 1.4 | Schematic diagram of FT–Raman spectrometer | 10 |
| Figure 1.5 | Schematic diagram of Nd:YAG laser | 11 |
| Figure 1.6 | Polarisation of a $p$–orbital by mixing with a $d$–function | 35 |
| Figure 1.7 | Morse potential energy surface | 38 |
| Figure 1.8 | Scaling factors and uncertainties | 39 |
| Figure 2.1 | Potential energy surface of (a) DOLOX, (b) DOLMX and (c) DOLPX calculated by B3LYP/6–31G method | 47 |
| Figure 2.2 | The most stable geometry, structure and atom numbering of $a,a'$–dil–o–xylene | 48 |
| Figure 2.3 | The most stable geometry, structure and atom numbering of $a,a'$–dil–m–xylene | 49 |
| Figure 2.4 | The most stable geometry, structure and atom numbering of $a,a'$–dil–p–xylene | 49 |
| Figure 2.5 | Temperature dependence of entropy of (a) DOLOX (b) DOLMX and (c) DOLPX | 53 |
| Figure 2.6 | Temperature dependence of heat capacity at constant pressure of (a) DOLOX (b) DOLMX and (c) DOLPX | 53 |
| Figure 2.7 | Temperature dependence of enthalpy change of (a) DOLOX (b) DOLMX and (c) DOLPX | 54 |
| Figure 2.8 | The molecular electrostatic potential surface of (a) DOLOX (b) DOLMX and (c) DOLPX | 55 |
| Figure 2.9 | The contour map of molecular electrostatic potential surface of (a) DOLOX (b) DOLMX and (c) DOLPX | 56 |
Figure 2.10  The frontier molecular orbitals of (a) DOLOX (b) DOLMX and (c) DOLPX

Figure 2.11  FTIR spectra of (a) α,α’–diol–o–xylene (b) α,α’–diol–m–xylene and (c) α,α’–diol–p–xylene

Figure 2.12  FT–Raman spectra of (a) α,α’–diol–o–xylene (b) α,α’–diol–m–xylene and (c) α,α’–diol–p–xylene

Figure 2.13  The linear regression between the experimental and theoretical scaled wavenumbers of (a) α,α’–diol–o–xylene, (b) α,α’–diol–m–xylene and (c) α,α’–diol–p–xylene

Figure 3.1  Possible conformers of α,α’–dibromo–o–xylene

Figure 3.2  Possible conformers of α,α’–dibromo–m–xylene

Figure 3.3  Possible conformers of α,α’–dibromo–p–xylene

Figure 3.4  The most stable geometry, structure and atom numbering of α,α’–dibromo–o–xylene

Figure 3.5  The most stable geometry, structure and atom numbering of α,α’–dibromo–m–xylene

Figure 3.6  The most stable geometry, structure and atom numbering of α,α’–dibromo–p–xylene

Figure 3.7  The molecular electrostatic potential surface of (a) DBOX (b) DBMX and (c) DBPX

Figure 3.8  The contour map of molecular electrostatic potential surface of (a) DBOX (b) DBMX and (c) DBPX

Figure 3.9  Electrostatic potential surface of (a) DBOX (b) DBMX and (c) DBPX

Figure 3.10  FTIR spectra of (a) α,α’–dibromo–o–xylene (b) α,α’–dibromo–m–xylene and (c) α,α’–dibromo–p–xylene

Figure 3.11  FT–Raman spectra of (a) α,α’–dibromo–o–xylene (b) α,α’–dibromo–m–xylene and (c) α,α’–dibromo–p–xylene
Figure 3.12 The linear regression between the experimental and theoretical scaled wavenumbers of (a) α,α′-dibromo-o-xylene, (b) α,α′-dibromo-m-xylene and (c) α,α′-dibromo-p-xylene

Figure 4.1 Atom numbering of (a) 4-methyl-1,3-dioxolan-2-one and (b) 4,5-dichloro-1,3-dioxolan-2-one

Figure 4.2 The molecular electrostatic potential surface of (a) 4,5-dichloro-1,3-dioxolan-2-one and (b) 4-methyl-1,3-dioxolan-2-one

Figure 4.3 The contour map of molecular electrostatic potential surface of (a) 4,5-dichloro-1,3-dioxolan-2-one and (b) 4-methyl-1,3-dioxolan-2-one

Figure 4.4 Electrostatic potential surface of (a) 4,5-dichloro-1,3-dioxolan-2-one and (b) 4-methyl-1,3-dioxolan-2-one

Figure 4.5 FTIR and FT–Raman spectrum of 4-methyl-1,3-dioxalan-2-one

Figure 4.6 FTIR and FT–Raman spectrum of 4,5-dichloro-1,3-dioxalan-2-one

Figure 5.1 Potential energy surface of 2-chloro-4-methyl-3-nitropyridine calculated by B3LYP/6–31G method

Figure 5.2 Potential energy surface of 2-chloro-6-methylpyridine calculated by B3LYP/6–31G method

Figure 5.3 The most stable geometry, structure and atom numbering of 2-chloro-4-methyl-3-nitropyridine

Figure 5.4 The most stable geometry, structure and atom numbering of 2-chloro-6-methylpyridine

Figure 5.5 Temperature dependence of entropy of 2-chloro-4-methyl-3-nitropyridine (2C4M3NP) and 2-chloro-6-methylpyridine (2C6MP)
Figure 5.6 Temperature dependence of heat capacity at constant pressure of 2–chloro–4–methyl–3–nitropyridine (2C4M3NP) and 2–chloro–6–methylpyridine (2C6MP)

Figure 5.7 Temperature dependence of enthalpy change of 2–chloro–4–methyl–3–nitropyridine (2C4M3NP) and 2–chloro–6–methylpyridine (2C6MP)

Figure 5.8 The total electron density isosurface mapped with molecular electrostatic potential of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 5.9 The contour map of molecular electrostatic potential surface of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 5.10 The frontier molecular orbitals of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 5.11 FTIR spectra of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 5.12 FTIR spectra of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 5.13 The linear regression between the experimental and theoretical scaled wavenumbers of (a) 2–chloro–4–methyl–3–nitropyridine and (b) 2–chloro–6–methylpyridine

Figure 6.1 Atom numbering scheme of 2–chloro–1H–isoindole–1,3(2H) dione (X = Cl) and 2–methyl–1H–isoindole–1,3(2H)–dione (X = –CH3)

Figure 6.2 Molecular structure of (a) 2–methyl–1H–isoindole–1,3(2H)–dione and (b) 2–chloro–1H–isoindole–1,3(2H)–dione

Figure 6.3 The total electron density isosurface mapped with molecular electrostatic potential of (a) 2–methyl–1H–isoindole–1,3(2H)–dione and (b) 2–chloro–1H–isoindole–1,3(2H)–dione

Figure 6.4 The contour map of molecular electrostatic potential surface of (a) 2–methyl–1H–isoindole–1,3(2H)–dione and
(b) 2-chloro-1H-isoindole-1,3(2H)-dione

Figure 6.5 Electrostatic potential surface of (a) 2-methyl-1H-
isoindole-1,3(2H)-dione and (b) 2-chloro-1H-
isoindole-1,3(2H)-dione

Figure 6.6 FTIR spectrum of 2-chloro-1H-isoindole-1,3(2H)-dione
(a) Observed (b) Calculated

Figure 6.7 FT-Raman spectrum of 2-chloro-1H-isoindole-1,3(2H)-
dione (a) Observed (b) Calculated

Figure 6.8 FTIR spectrum of 2-methyl-1H-isoindole-1,3(2H)-dione
(a) Observed (b) Calculated

Figure 6.9 FT-Raman spectrum of 2-methyl-1H-isoindole-
1,3(2H)-dione (a) Observed (b) Calculated

Figure 7.1 Structure and atom numbering scheme of 4-amino-2-
methylquinoline

Figure 7.2 The total electron density isosurface mapped with
molecular electrostatic potential of 4-amino-2-
methylquinoline

Figure 7.3 Electrostatic potential surface of 4-amino-2-
methylquinoline

Figure 7.4 The contour map of molecular electrostatic potential
surface of 4-amino-2-methylquinoline

Figure 7.5 FTIR spectrum of 4-amino-2-methylquinoline
(a) Observed (b) Theoretical HF/6-311++G** and
(c) B3LYP/6-311++G**

Figure 7.6 FT-Raman spectrum of 4-amino-2-methylquinoline
(a) Observed (b) Theoretical HF/6-31G** and (c) HF/
6-311++G**