CHAPTER-4
X-Ray K-absorption
spectral studies of Copper (II) complexes
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References
4.1 Introduction

X-ray absorption fine structure (XAFS) spectroscopy becomes a powerful technique providing analytical as well as structural information, with applications in a wide range of scientific fields because of the rapid development of the data treatment techniques. Synchrotron X-ray absorption fine structure spectroscopy is an effective technique for selectively investigating the local coordination environment of metal ions [1-3].

Copper is chemical element with the symbol Cu and atomic number 29. It is a ductile metal, with very high thermal and electrical conductivity. Pure copper is rather soft and malleable, and a freshly exposed surface has a reddish-orange colour. It is used as a thermal conductor, an electrical conductor, a building material, and a constituent of various metal alloys. It has face-centred cubic crystalline structure. It reflects red and orange and absorbs other frequencies in the visible spectrum, due to its band structure, so it has a nice red colour. Copper has low chemical reactivity. It is more commonly encountered in everyday life. For instance, it is applied in the industries and in agriculture. The production of copper has lifted over the last decades. Copper can be released into the environment by both natural sources and human activities.

Pyrazole derivatives exhibit important biological properties such as antitumour [4], anticoagulant [5], and antihyperglycemic, analgesic, anti-inflammatory, anti-pyretic, antibacterial, hypoglycemic and sedative–hypnotic activity [6–8]. These derivatives have attracted significant attention because of the application in drug development [9].

Macrocyclic complexes are involved in important biological processes, such as photosynthesis and dioxygen transport in addition to their catalytic properties [10] which may lead to important industrial applications. Their enhanced kinetic and thermodynamic stabilities led to a widespread study of the features which also influence their potential applications as metal extractants [11] and as radiotherapeutic [12] and medical imaging agents. Due to importance in biological systems and as a synthetic model for many metalloenzyme reactions [13-15], their novel structural features, and unusual magnetic properties.
XAFS experiment has been performed at the K-edge of copper in the complex at the dispersive EXAFS beamline at 2 GeV Indus-2 synchrotron source at RRCAT, Indore, India.

The proposed method has been applied to the following two series of copper complexes.

1. Three copper (II) complexes having pyrazole as a ligand (series-I).
2. Five copper macrocyclic complexes (Series-II).

4.2 Experimental

The X-ray absorption spectra at the K-edge of copper of complexes have been recorded at the Dispersive Extended X-ray Absorption Fine Structure (DEXAFS) beamline, which has been recently set-up by Applied Spectroscopy Division, BARC at the Indus-2 synchrotron radiation source at Raja Ramanna Centre for Advanced Technology (RRCAT), Indore [16-18].

The detailed description of the Dispersive Extended X-ray Absorption Fine Structure (DEXAFS) Beamline (BL-8) has already been given in chapter II of this thesis.

4.3 Results

In an XAFS experiment the incident and transmitted X-ray intensities are measured as a function of energy. The intensity of the x-ray after passing through a sample of thickness x is given by: \( I_t = I_0 e^{-\mu x} \), where \( \mu \) is the absorption coefficient and \( x \) is the thickness of the absorber, the absorption \( \mu(E) \) corresponding to the photon energy \( E \).

The plot of absorption versus photon energy is obtained by recording the intensities \( I_0 \) and \( I_t \), as the CCD outputs, without and with the sample, respectively, and the absorption coefficient \( \mu \) is obtained using above relation. The experimental data has been analyzed using the available computer software package Athena version 0.8.061. The various steps of the procedure of the analysis are given in figures 4.1 (for Cu metal), 4.2- 4.4 (for series-I copper complexes) and 4.5- 4.9 (for series-II copper complexes).

The absorption spectra of the copper metal and its complexes are shown in figure 4.1 (a), 4.2-4.4 (a) and 4.5-4.9 (a). The normalization process has already been described in previous chapter of this thesis. Figures 4.1 (b), 4.2-4.4 (b) and 4.5- 4.9 (b) shows the smooth polynomial spline has been fitted to the XAFS to...
remove the slowly varying (low-frequency) components of $\mu(E)$. Figures 4.1 (c), 4.2-4.4 (c) and 4.5-4.9 (c) shows that the normalized absorption spectra with the pre-edge along zero, an edge step of one and the post-edge region oscillating around one for copper metal, series-I and series-II copper complexes.

4.3.1 The absorption edge

Figures 4.1 (d), 4.2-4.4 (d) and 4.5-4.9 (d) indicating the positions of the absorption edge K and principal absorption maximum A in the region $-30 < E < 50$ eV of all copper complexes, in XAFS spectra. The values of $E_K$ for the K-absorption edge of copper metal and its complexes studied are given in table 4.1. These have been determined as the energies of the first peak in the derivative spectra.

4.3.2 Position of the edge

In the region $30 < E < 50$ eV, figures 4.1 (e), 4.2-4.4 (e) and 4.5-4.9 (e) shows that the first derivative of absorption spectra indicating the position of the absorption edges K and principal absorption maximum A. The K-absorption edge ($E_K$) described by the first peak i.e., the position of first inflection point in the derivative spectra. The position where the derivative is zero, gives the position of principal absorption maxima ($E_A$). The results of the energies of the K-absorption edge ($E_K$) and the energies of principal absorption maximum A ($E_A$) of copper in metal and its complexes are presented in table 4.1.

Figures 4.1 (f), 4.2-4.4 (f) and 4.5-4.9 (f) shows that the EXAFS spectra converted into k space. The maxima and minima of the spectra for different values of k have been labelled with the conventional Latin and Greek alphabets respectively. The values of energy E and wave vector k corresponding to these maxima and minima have been given in table 4.2 for copper metal and copper (II) complex of series-I and series-II.

4.3.3 Chemical shift

The K-absorption edge of copper has been found to be shifted towards the high energy side in all the complexes, as compared to the K-absorption edge in the copper metal. The shifts of the K-absorption edge of copper in the complexes with respect to that of copper metal have been determined according to the eqn. $\Delta E_K = E_K (\text{complex}) - E_K (\text{metal})$. The chemical shifts (in eV) of the K-absorption edge of copper in the complexes are given in table 4.1. For computing the chemical
shift the value of $E_K$ (Cu metal) has been taken as 8979.27 eV. The order of the chemical shifts as indicated by their values from table 4.1 has been found to be as follows:

**Series-1**

Cu (D4A1(3-Cl)1HP35D) > Cu (D4A1(2-N)1HP35D) > Cu (D4A1(P-N)1HP35D)

**Series-2**

Cu (C16H10N2O6) > Cu (C24H26N206) > Cu (C28H18N206) >

Cu (C20H18N2O6) > Cu (C18H14N2O6)

The compounds having copper in oxidation state in +1 show chemical shifts less than 5 eV while those having copper in oxidation state in +2 show chemical shifts more than 5 eV [19]. In table 4.1, all the complexes have the values of chemical shifts between 7.36-8.75 eV for series-I copper complexes and 7.53 - 8.84 eV for series-II copper complexes. Hence, on the basis of values of the chemical shifts, all the complexes (series-I and series-II) are found to have copper in oxidation state +2.

As is well known, the chemical shift reflects the ionic character of the complex, more the chemical shift, more the ionic character. As the complexes Cu (D4A1(3-Cl)1HP35D) and Cu (C16H10N2O6) is showing highest chemical shift in the above series (series-I and II), hence, it should have the maximum ionic character amongst the studied complexes.

### 4.3.4 Principal absorption maximum

The principal absorption maximum $A$ with respect to the respective K-absorption edge of all copper complexes are also given in table 4.1. It has been shown that the value of $E_A$ of complexes is shifted towards the higher energy side with respect to copper metal. The reason for the shift of the principal absorption maximum to the higher energy side has already been discussed in previous chapter.

For the complexes mentioned in table 4.1, the energy range of chemical shift in copper complexes is between 7.36 - 8.75 eV for series-I complexes and 7.53 - 8.84 eV for series-II complexes while the range for shift of principal absorption maximum is between 18.5 – 19.31 eV for series-I complexes and 19.52- 21.39 eV for series-II. Hence, on the basis of the shift of the principal absorption maximum also it can be inferred that copper is in +2 oxidation state in
these complexes. The order of shift of the principal absorption maximum in the copper complexes is as follows:

**Series-I**

Cu (D4A1(3-Cl)1HP35D) < Cu (D4A1(2-N)1HP35D) < Cu (D4A1(P-N)1HP35D)

**Series-II**

Cu (C16H10N2O6) < Cu (C24H26N2O6) < Cu (C28H18N2O6) <

Cu (C20H18N2O6) < Cu (C18H14N2O6)

The order of shift of principal absorption maximum is in reverse order of the chemical shift for all copper complexes. The reverse order represents that the shift of A is inversely proportional to ionic character for both series copper complexes.

### 4.3.5 Edge-width

In table 4.1, the values of the edge-width (E_A - E_K) have been reported. The edge-width data for the copper complexes is as follows:

**Series-I**

Cu (D4A1(3-Cl)1HP35D) < Cu (D4A1(2-N)1HP35D) < Cu (D4A1(P-N)1HP35D)

**Series-II**

Cu (C16H10N2O6) < Cu (C24H26N2O6) < Cu (C28H18N2O6) <

Cu (C20H18N2O6) < Cu (C18H14N2O6)

The order of the edge-width is in the reverse order of chemical shift of the complexes. The reverse order represents that the edge-width is inversely proportional to ionic character for this series. The edge-width of the K-absorption edges increase with the increase in covalent character of the bonds provided other factors like molecular geometry etc. remain the same [20]. In the present work, edge-width of copper complexes is observed to vary from 7.36 - 8.75 eV for series-I complexes and 10.68 – 13.86 eV for series-II complexes.

### 4.3.6 Determination of bond lengths

(i) **By graphical methods from EXAFS spectra**

The EXAFS appearing on high energy side of the K-absorption edge have been recorded in all the copper complexes. Following the principal absorption maxima, there are distinct EXAFS features, extending up to 300 eV on the high energy side of the K-absorption edge. The K-absorption discontinuity along with
fine structure for all the complexes are shown in figures 4.1 (a), 4.2-4.4 (a) and 4.5-4.9 (a).

In the XAFS spectra, the inflection point on the K-absorption edge is taken as the reference point for the measurement of the extended fine structure. The positions of the EXAFS maxima and minima in eV and their corresponding values of k in Å⁻¹ are given in table 4.2.

The Fourier transformation technique can be used for determination of the bond lengths. The magnitudes of Fourier transform of copper metal and its complexes are shown in figures 4.1 (g), 4.2-4.4 (g) for series-I complexes and 4.5-4.9 (g) for series-II complexes and the calculated bond lengths have been shown in table 4.3. This bond length also known as phase uncorrected bond length, i.e., R₁-α₁.

The bond length can also be determined from EXAFS data by three graphical methods i.e., Levy’s, Lytle’s and Lytle, Sayers and Stern’s (L.S.S.) methods. These methods are briefly mentioned below. Infect, before the Fourier transformation technique was formulated, the bond length used to be extracted from the EXAFS data by these three methods. We have used all the three methods for determination of bond lengths in cobalt complexes studied in the present chapter. The bond lengths determined for the cobalt complexes with the help of three methods are given in table 4.3.

(A) **Levy’s method**

It is simple method of determining bond length, according to it the bond lengths are calculated by using the eq.

\[ R₁ = \left[ \frac{151}{ΔE} \right]^{1/2} \text{Å}, \]

Where ΔE is the difference of the energies of the EXAFS maximum B and minimum β and R₁ is the radius of the first coordination sphere. The positions of B and β are given in table 4.2 for the complexes. The bond lengths thus determined are given in table 4.3 [21].

(B) **Lytle’s method**

The energy values (E) of the EXAFS maxima, given in table 4.2, are plotted against the Q values given by Lytle, i.e., Q = 2.04, 6.0, 12.0, and 20.0. The (E, Q) plots have been found to be linear and are given in figures 4.10 and 4.11.
The slopes $M$ of the $E$ versus $Q$ plots have been used to evaluate the radius $R_s$ of equivalent polyhedron, by using the relation:

$$R_s = \left( \frac{37.60}{M} \right)^{1/2}$$

The values of $R_s$ calculated with the help of this method are reported in table 4.3 for all the complexes [22].

(C) **L.S.S. method**

The values of the wave vector $k$ (Å$^{-1}$) for EXAFS maxima ($n = 0, 2, 4,...$) and minima ($n = 1, 3, 5,...$), for all the cobalt complexes, are presented in table 4.2. In the Lytle, Sayers and Stern's (L.S.S.) method for determination of the nearest neighbor distances, $n$ versus $k$ graph is plotted. The plots have been found to be linear for all the complexes and are shown in figures 4.12 and 4.13. The slope of $n$ versus $k$ plot, gives the value of $2(R_i - a_1) / \pi$, where $R_i$ is the bond length. The values of $(R_i - a_1)$ thus obtained are given in table 4.3 [23].

(ii) **By Fourier transform of EXAFS spectra**

The Fourier transform of the $\chi(k)$ versus $k$ spectra peaks at the radial distances of the neighboring atoms from the absorbing atom. However, the distance found from Fourier transform is about 0.2 Å - 0.5 Å shorter than the actual distance due to energy dependence of the phase factors in the sine function of the EXAFS. The peaks in the Fourier transform are shifted towards the origin by an amount $\alpha_i$ and hence the peaks are at distances $R_i - \alpha_i$ [24]. For the first peak $j=1$ and hence the position of the first peak determines the distance $R_i - \alpha_i$.

It is important to note here that the distance $R_i - \alpha_i$ should be equal to the distance found from the L.S.S. graphical method. Hence, both the L.S.S. method and the Fourier transformation method give the value $R_i - \alpha_i$, i.e., both the methods give the value of bond lengths which have not been corrected for the phase shifts. We have called this distance as the phase uncorrected bond length.

The normalized spectra are shown in figures 4.1 (c), 4.2-4.4 (c) and 4.5-4.9 (c) are $\mu(E)$ versus E curves obtained. From these curves, $\chi(k)$ versus $k$ curves are obtained which are given in figures 4.1 (f), 4.2-4.4 (f) and 4.5-4.9 (f). The Fourier transformed spectra obtained from $\chi(k)$ versus $k$ curves are given in figures 4.1 (g), 4.2-4.4 (g) and 4.5-4.9 (g). The position of the first peak in the Fourier transform gives the value of $R_i - \alpha_i$ and the values are collected in table 4.3 for all the complexes.
It is seen from table 4.3 that the value of $R_1-a_1$ as determined from L.S.S. method and that determined from the Fourier transformation method are in good agreement with each other, i.e., both the L.S.S. method and Fourier transformation method give nearly the same value of the phase uncorrected bond length, i.e., $R_1-a_1$.

### 4.4 Conclusions

The conclusions drawn in this chapter are as follows:

- X-ray absorption spectra of copper complexes at the K-edge of copper have been recorded at the recently developed EXAFS beamline set-up at the Indus-2 synchrotron source at RRCAT, Indore.
- The K-edge absorption edge has been found in all copper complexes. The energies of K-edge ($E_K$), the values of chemical shifts, the principal absorption maxima ($E_A$) and EXAFS maxima and minima have been reported.
- The shift of the K-edge (chemical shift) has been obtained for all copper complexes. All the complexes have the values of chemical shifts between 7.36-8.75 eV for series-I copper complexes and 7.53 - 8.84 eV for series-II copper complexes. The complexes Cu (D4A1(3-Cl)1HP35D) and Cu (C16H10N2O6) is showing highest chemical shift in the copper series (series-I and II ), hence, it should have the maximum ionic character amongst the studied complexes. The values of the chemical shifts suggest that copper is in oxidation state +2 in all of the complexes.
- The values of shift of the principal absorption maximum have been obtained for all copper complexes. The order of shift of principal absorption maximum for all the complexes is in reverse order of the chemical shift. The reverse order represents that the shift of the principal absorption maximum is inversely proportional to ionic character for the complexes. The complexes Cu (D4A1(P-N)1HP35D) and Cu (C18H14N206)is showing highest values of shift of principal absorption maxima for series-1 and series-2 complexes.
- The edge-width has also been studied for all the complexes. The order of the edge-width is in the reverse order of chemical shift of the complexes.
The reverse order represents that the edge-width is inversely proportional to ionic character for this series.

- From the positions of the EXAFS maxima and minima, the bond lengths in the complexes have been determined by three different methods viz. Levy's, Lytle's and Lytle, Sayers and Stern's (L.S.S.) methods.
- The normalized spectra, i.e., $\mu(E)$ versus $E$ curves have been obtained. From these curves, $\chi(k)$ versus $k$ curves have been obtained, which have then been Fourier transformed using the software Athena. From the Fourier transforms of the EXAFS spectra the bond lengths have been determined.
- It has been observed that the value of the phase uncorrected bond length, i.e., $R_1-\alpha_1$ as determined from L.S.S. method and that determined from the Fourier transformation method are in good agreement with each other, i.e., both the L.S.S. method and Fourier transformation method give nearly the same value of the phase uncorrected bond length.
<table>
<thead>
<tr>
<th>Complex</th>
<th>( E_k ) (eV)</th>
<th>( E_A ) (eV)</th>
<th>Chemical shift ( \Delta E_k = (E_{\text{complex}} - E_{\text{metal}}) ) (eV)</th>
<th>Shift of the principal absorption maximum (eV)</th>
<th>Edge-width ( (E_A - E_k) ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu metal</td>
<td>8979.27</td>
<td>9003.51</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>Cu(D4A1(3-Cl)1HP35D)</td>
<td>8988.02</td>
<td>8998.56</td>
<td>8.75</td>
<td>19.29</td>
<td>10.54</td>
</tr>
<tr>
<td>Cu(D4A1(2-N)1HP35D)</td>
<td>8987.03</td>
<td>8998.57</td>
<td>7.76</td>
<td>19.3</td>
<td>11.54</td>
</tr>
<tr>
<td>Cu(D4A1(P-N)1HP35D)</td>
<td>8986.63</td>
<td>8998.58</td>
<td>7.36</td>
<td>19.31</td>
<td>11.94</td>
</tr>
<tr>
<td>Cu (C16H10N2O6)</td>
<td>8988.11</td>
<td>8998.79</td>
<td>8.84</td>
<td>19.52</td>
<td>10.68</td>
</tr>
<tr>
<td>Cu (C24H26N2O6)</td>
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<td>8.51</td>
<td>20.06</td>
<td>11.55</td>
</tr>
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<td>Cu (C28H18N2O6)</td>
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<td>8999.85</td>
<td>8.11</td>
<td>20.58</td>
<td>12.47</td>
</tr>
<tr>
<td>Cu(C20H18N2O6)</td>
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<td>9000.43</td>
<td>7.94</td>
<td>21.16</td>
<td>13.22</td>
</tr>
<tr>
<td>Cu (C18H14N2O6)</td>
<td>8986.8</td>
<td>9000.66</td>
<td>7.53</td>
<td>21.39</td>
<td>13.86</td>
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</table>
Table 4.2: Energy $E$ (eV) and wave vector $k$ (Å$^{-1}$) for EXAFS maxima and minima at the K-absorption edge of cobalt (II) complexes and their corresponding values of $n$ and energy level $Q$.

<table>
<thead>
<tr>
<th>Structure</th>
<th>n</th>
<th>Q</th>
<th>$E$ (eV)</th>
<th>$k$ (Å$^{-1}$)</th>
<th>$E$ (eV)</th>
<th>$k$ (Å$^{-1}$)</th>
<th>$E$ (eV)</th>
<th>$k$ (Å$^{-1}$)</th>
<th>$E$ (eV)</th>
<th>$k$ (Å$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0</td>
<td>2.04</td>
<td>12.31</td>
<td>1.85</td>
<td>13.01</td>
<td>1.9</td>
<td>13.01</td>
<td>1.85</td>
<td>12.31</td>
<td>1.8</td>
</tr>
<tr>
<td>a</td>
<td>1</td>
<td>-</td>
<td>41.40</td>
<td>3.3</td>
<td>41.40</td>
<td>3.3</td>
<td>41.40</td>
<td>3.3</td>
<td>41.40</td>
<td>3.3</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
<td>6.04</td>
<td>67.07</td>
<td>4.2</td>
<td>68.67</td>
<td>4.25</td>
<td>67.07</td>
<td>4.2</td>
<td>67.70</td>
<td>4.2</td>
</tr>
<tr>
<td>β</td>
<td>3</td>
<td>-</td>
<td>108.83</td>
<td>4.35</td>
<td>108.83</td>
<td>4.35</td>
<td>108.83</td>
<td>4.35</td>
<td>110.87</td>
<td>4.4</td>
</tr>
<tr>
<td>C</td>
<td>4</td>
<td>12.0</td>
<td>160.64</td>
<td>6.5</td>
<td>160.64</td>
<td>6.5</td>
<td>160.64</td>
<td>6.5</td>
<td>163.12</td>
<td>6.55</td>
</tr>
<tr>
<td>γ</td>
<td>5</td>
<td>-</td>
<td>202.62</td>
<td>7.3</td>
<td>197.11</td>
<td>7.2</td>
<td>199.84</td>
<td>7.25</td>
<td>202.62</td>
<td>7.3</td>
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Table 4.3: Values of first shell bond lengths (in Å) calculated from Levy’s, Lytle’s, L.S.S. and Fourier transform methods for copper (II) complexes

<table>
<thead>
<tr>
<th>S.No.</th>
<th>Complex</th>
<th>Phase corrected</th>
<th>Phase uncorrected</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Levy’s method</td>
<td>Lytle’s method</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$R_1$</td>
<td>$R_s$</td>
</tr>
<tr>
<td>1</td>
<td>Cu(D4A1(3-Cl)1HP35D)</td>
<td>1.89</td>
<td>1.58</td>
</tr>
<tr>
<td>2</td>
<td>Cu(D4A1(P-N)1HP35D)</td>
<td>1.99</td>
<td>1.58</td>
</tr>
<tr>
<td>3</td>
<td>Cu(D4A1(2-N)1HP35D)</td>
<td>1.98</td>
<td>1.57</td>
</tr>
<tr>
<td>4</td>
<td>Cu (C24H26N2O6)</td>
<td>1.93</td>
<td>1.6</td>
</tr>
<tr>
<td>5</td>
<td>Cu (C18H14N2O6)</td>
<td>1.87</td>
<td>1.57</td>
</tr>
<tr>
<td>6</td>
<td>Cu (C16H10N2O6)</td>
<td>1.9</td>
<td>1.58</td>
</tr>
<tr>
<td>7</td>
<td>Cu (C28H18N2O6)</td>
<td>1.97</td>
<td>1.59</td>
</tr>
<tr>
<td>8</td>
<td>Cu (C20H18N2O6)</td>
<td>1.85</td>
<td>1.57</td>
</tr>
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</table>
Figure: 4.1(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu metal.
Figure: 4.1 (e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus k curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus k curve for Cu metal.
Figure: 4.2 (a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu (D4A1(2-N)1HP35D).
Figure: 4.2(e) Derivative of XAFS spectrum for Cu metal position of absorption edges KI and principal absorption maxima A. (f) $\chi(k)$ versus k curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus k curve for Cu(D4A1(2-N)1HP35D).
Figure: 4.3(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu(D4A1(3-Cl)1HP35D).
Figure: 4.3(e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus k curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus k curve for Cu(D4A1(3-Cl)1HP35D).
Figure: 4.4(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu(C24H26N2O6).
Figure: 4.4(e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) \( \chi(k) \) versus k curve and (g) Magnitude of Fourier transform of the \( \chi(k) \) versus k curve for Cu(C24H26N2O6).
Figure: 4.5(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu (C18H14N2O6).
Figure: 4.5(e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus k curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus k curve for Cu (C18H14N2O6).
Figure: 4.6(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu (C16H10N2O6).
Figure: 4.6(c) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus $k$ curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus $k$ curve for Cu (C16H10N2O6).
Figure: 4.7(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu(D4A1(P-N)1HP35D).
Figure: 4.7(e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus k curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus k curve for Cu(D4A1(P-N)1HP35D).
Figure: 4.8(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu \((\text{C}_2\text{H}_{18}\text{N}_2\text{O}_6)\).
Figure: 4.8(e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus $k$ curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus $k$ curve for Cu (C28H18N2O6).
Figure: 4.9(a) Raw absorption versus photoelectron energy (b) Absorption with smooth background function (c) The normalized absorption spectrum and (d) XAFS spectrum for Cu (C20H18N2O6).
Figure: 4.9 (e) Derivative of XAFS spectrum for Cu metal position of absorption edges K1 and principal absorption maxima A. (f) $\chi(k)$ versus $k$ curve and (g) Magnitude of Fourier transform of the $\chi(k)$ versus $k$ curve for Cu (C20H18N2O6).
Figure: 4.10 (a) E versus Q curves for the copper (II) complexes (series-I).
Figure: 4.11 E versus Q curves for the copper (II) complexes (series-I).
Figure: 4.12 $n$ versus $k$ curves for the copper (II) complexes (series-I).
Figure: 4.13 $n$ versus $k$ curves for the copper (II) complexes (series-II).
References


