Exafs data analysis of some cobalt complexes

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Abstract. X-ray spectroscopy has assumed great significance with its increasing application in the different fields of physics like solid state physics, chemical physics, atomic physics, Plasma Physics and Astro physics etc. in present paper we obtained bond lengths of cobalt metal complexes using Levy’s, LSS and Lytle methods and are compared by FEFFIT (Fitting of EXAFS by Fast Fourier Inverse Transform) method. Bond length basically known as radial distance between ligand and metal complexes. FEFFIT is computer program for calculating bond length obtained theoretical data of EXAFS.

1.Introduction
Present paper deals with analysis of bond length calculation by EXAFS study. In the absorption edges, EXAFS ranging from 50 to about 1000eV above the edge. Lytle, Sayers and Stern related these fluctuations of the absorption coefficient to the atomic arrangement surrounding of the absorbing atom. Structural information is obtained from EXAFS either by a comparison of an unknown compound with a known model. With help of EXAFS using IFEFFIT method we are find the bond lengths and structural characteristics of Cobalt complexes [1] We have used Cobalt amino acid complexes for X-ray absorption fine structure studies are- 1.Cu-Aspartic acid, and 2.Cu-Glutamic acid. Amino acids are critical to life, and have many functions in metabolism. One particularly important function is to serve as the building blocks of proteins, which are linear chains of amino acids. Cobalt is a member of first transition series elements that have been of particular interest, for the possibility of various valance states is always there due 3d incomplete shell. The electronic configuration of cobalt is (A) 3d7 4s2. Cobalt compounds are widely used to make coloring materials the transition metals are capable of showing several oxidation states. The members of the first transition series form more stable complexes with ligands congaing nitrogen and oxygen while the members of the complexes. One of the most important properties of transition elements from s and p-block elements is that they show variable oxidation states. When an X-ray beam passes through a material, its intensity falls off according to the relation

\[ I(x) = I_0 e^{-\mu x} \]

where \( I_0 \) is the intensity of X-rays incident on the material, \( I \) is the intensity at a distance \( x \) in the material and \( \mu \) is the linear absorption coefficient. [2]

The physics of EXAFS, was originally explained by the short range order theory of Kronig in 1932 [3-4], and confirmed experimentally by Sayers, Lytle, and Stern in 1971 [5]. In this region photo-electrons have sufficient energy to effectively propagate through the sample as free particles. Extended X-ray absorption fine structure (EXAFS) spectroscopy has been a valuable probe of local structure in molecules, surfaces, and solids.
2. Experimental details

The X-ray generator manufactured by Messrs. Rich Seifert and Co., Germany, was used for the production of X-rays. Its principle components are: X-ray tube housing type SN60, High voltage generator and control module basic equipment n.ID 3000, & Water cooling system no. KKS3.

X-ray absorption edge studies were carried out using a conventional Siefert sealed X-ray tube with Tungsten target operating at 20 kV and 40 mA. After this process, the X-ray films were completed on Carl-Ziess Microdensitometer coupled with a computer to convert the data into IFEFFIT analysis.

3. Results and Discussion

3.1. Extended X-ray Absorption fine structure

The bond lengths of cobalt complexes were calculated with IFEFFIT method, after this process, it has been compared with these three different methods.

1. Levy’s method.
2. LSS method
3. Lytle method

According to Levy’s method bond length given by \( R = (151/ \Delta E)^{1/2} \) where, \( \Delta E \) is the energy separation between first maxima and first minima. The LSS method is a graphical method and according to this method, the simplified equation for wave vector is given by \( k = (0.263E)^{1/2} \) where, \( E \) is energy position of different maxima and minima in fine structure curve measured from point in K-absorption edge. The total phase shift \( \delta_j(k) \) parameter was also determined using the expression \( \delta_j(k) = -\alpha_j k + \beta_j \cdot 1/2\Pi \), where notations have their usual meaning. Lytle method is modification of LSS method is given by the expression \( R = (37.60/M)^{1/2} \) Where \( M \) is slope Between \( E \) verses \( Q \) plots. The absorption energy maxima are \( E=A \), \( B \), \( C \), \( D \) and \( Q=2.4 \), \( 6.4 \), \( 12 \), \( 20 \) are constant.

Table 1. The bond length in (Å) of Cobalt complexes is calculated by FEFFIT programming and it compared by LSS, Levy’s, and Lytle methods.

| Cobalt complex | \( R_{\text{LSS}} \) | \( R_{\text{Lyte}} \) | \( R_{\text{LSS}} \) | \( R_{\text{IFEFFIT}} \) |
|----------------|-------------------|-------------------|-------------------|-------------------|
| Complexe1      | 1.47              | 1.40              | 1.58              | 1.21              |
| Complexe2      | 1.28              | 1.44              | 1.51              | 1.57              |

Figure 1: Magnitude of Fourier transform for Cobalt complex obtained from ATHENA program.
Figure 2: EXAFS function for Cobalt complex obtained from ATHENA program.

4. Conclusion
Here we have compared the bond lengths of Cobalt complex experimentally by LSS, Levy’s, and Lytle methods and we have also calculated theoretically by FEFFIT (ATHENA) programming. The calculated EXAFS curves for Co complexes are in good agreement with experimental EXAFS curves for all Cobalt complex studied within experimental error.

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