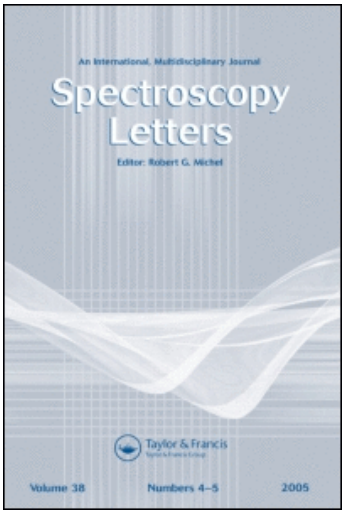

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Studies on the Photoacoustic Spectrum of Crystal of an Amino-Acid Copper Complex [Cu(L-Phe)(O-Phen)(H_2O)]NO_3-H_2O

Jianmin Li[a]; Ming Xu[a]; Min Yang[a]; Yugeng Zhang[a]
[a] Department of Chemical Physics, University of Science and Technology of China, IIeifei, Anhui, P. R. China

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Studies on the Photoacoustic Spectrum of Crystal of an Amino-Acid Copper Complex [Cu(L-Phe)(O-Phen)(H_2O)]$NO_3 \cdot H_2O$

Li Jianmin, Xu Ming, Yang Min, Zhang Yugeng

Department of Chemical Physics,University of Science and Technology of China,Heifei,Anhui, 230026,P.R.China

ABSTRACT:

Crystal of an amino-acid copper complex [Cu(L-Phe)(O-Phen)(H_2O)]NO_3 H_2O was synthesized, and its photoacoustic spectrum was recorded under room temperature. A semi-empirical method of coordinate-field theory was utilized to calculate the d-d transition energy. With the results, we explained the spectrum satisfactorily.

INTRODUCTIONS:

Metal proteins are of great significance in life activities. Many metal proteins act as high selective,high efficient catalysts in biological processes in living bodies[1].Other metal proteins (like *ferrohemoglobin*)are *good oxygen support* in *respirations*.As simple models of metal proteins, many amino-acid metal complexes are synthesized and researched[2][3].

In recent years,photoacoustic measurements have been widely used to investigate the chemical and physical properties of almost all kinds of samples,the precedence lies in that it enables the scientists to obtain spectrums of any type of solids,whether it is

crystalline, powder or gel. Theoretically, if the sample is not luminescent, the photoacoustic spectrum will coincide with the electronic absorption spectrum.

EXPERIMENTAL:

The object complex was synthesized according to a method submitted by Ref[5]. Photoacoustic spectrum was recorded in the region 300-800nm under room temperature, the excitation source was a 500W xenon lamp. The light source was modulated by a variable speed mechanical chopper at a frequency of 12HZ. The acoustic signal was detected with the sample placed in a locally built photoacoustic cell fitted with an ERM10 electret microphone.The output signal was normalized for changes in lamp intensity using a carbon-blank reference.

RESULTS AND DISCUSSIONS:

1.Description of the molecular structure:

The space coordinate condition of [Cu(L-Phe)(O-Phen)(H_2O)] $NO_3 \cdot H_2O$ is shown in Figure[1].To make it convenient in theoretical calculation,we describe the structure in a pole coordinate system ,the values are given in Table1.

2.Theoretical calculation and spectrum resolution

The photoacoustic spectrum is given in Figure[2].We can see a broad intense peak in 16050cm^{-1} and a relatively sharp peak in 30300cm^{-1}.

Firstly,there is a relatively sharp peak in near ultraviolet region,the researches on the photoacoustic spectrum suggest that it is not a ultraviolet absorption of the π obital absorption of the ligands.We attribute this peak to the LMCT transition from the π obitals of the ligands to the d obitals of central ion Cu(II) [6]. We attibute the broad intense peak in 16050cm^{-1} to the d obitals electronic transition of the central ion Cu(II). The

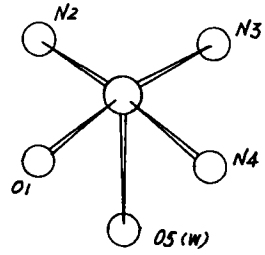

Fig. 1. Simplified space structure

TABLE 1

The data of the crystal structure of $[Cu(L\text{-}ArgH)_2(Ac)_2]3H_2O$

R,θ,φ	O(1)	N(2)	O(3)	N(4)	O(5)
R(Å)	1.927	2.004	2.010	1.968	2.213
θ(deg.)	103.9	96.4	92.4	94.1	0
φ(deg.)	189.7	261.8	0	82.9	/

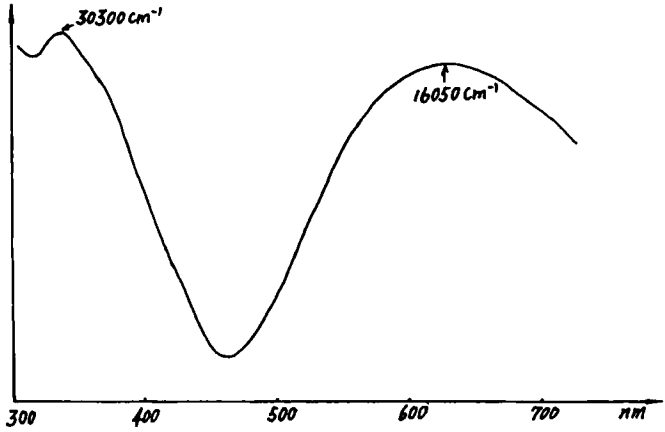

Fig. 2. Photoacoustic spectrum

TABLE 2

Values of d-d transition energy(unit:cm^{-1})

Peak	transition energy value
ν_1	7019
ν_2	12830
ν_3	14542
ν_4	16995

spectrum is not sharp peaks caused by split d-d energy gap as we anticipated. It is caused by the following reasons:1.Crystal grating vibrations. The vibrations make the distances between the central ions and the coordinate atoms change quickly in a certain region, which makes the coordinate field intensity change in a certain region. 2.Jahn-Teller effect. 3.The low symmetry of the coordinate field makes the d energy level split.It is necessary to explain the spectrum in details.We now utilize a semi-empirical method PLFT[7-11] of the coordinate field theory to calculate the d energy level.

PLFT is such a software pack: Point electric charge-electric dipole model are adopted; Under central-force field approximation, radial wave functions of non-freedom transition-metal ions are determined. With strong-field disposal of the coordinate theory, FORTRAN77 structural language is utilized to write the software. In this software there is only one adaptable parameter-the convalency factor $\bar{N}^2$, which is between 0.8 to 1.0. So far the software pack has successfully explained spectrum properties of more than one hundred transition-metal complex crystals[4].

The parameters of the crystal field and electronic energy level are calculated and the the values are shown in Table 2.

Electronic absorption spectrums of other amino acid-copper complexes were studied[12].It was concluded that the intensity and

the position of the broad peak are generally determined by ν_3 and ν_4 transitions, which coincides with our results:The position of the broad peak 16050cm^{-1} is just between ν_3(14542cm^{-1}) and ν_4(16995cm^{-1}). The photoacoustic spectrum is satisfactorily explained. Ref[13] assumed transitions ν_1 and ν_2 are determined by a certain space inhibition, so far the assumption has not been proved theoretically.In fact,the intensity distribution of the d-d electronic transition has not been explained by a successful theory.

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