The Possibility of Electronic Spectra Utilization for Molecular Structure Determination in the Case of Cu(II) Complexes with 2,2'-Bipyridyl and *o*-Phenanthroline

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In several papers dealing with Cu(II) coordination compounds with chelate ligands it was stated that electronic spectra could be used to find the stereochemistry of Cu(II) complexes [1–5]. However, it was also shown that such kind of determinations are not unambiguous [6].

We have prepared and studied the compounds with the composition Cu(o-phen)$_2$(NCS)$_2$ and Cu(o-phen)$_2$(NCSe)$_2$ (o-phen = 1,10-phenanthroline) [7]. The X-ray structure investigation results help to solve the problem of the utilization of the absorption electronic spectra for their molecular structure determination.

It was found that both of above compounds are isostructural (space group Pbcn, Z = 4). The molecular structure of Cu(o-phen)$_2$(NCSe)$_2$ is shown in Fig. 1.

The crystal structure consists of neutral complex molecules of the composition Cu(o-phen)$_2$(NCX)$_2$ (X = S, Se) which are held together by van der Waals interactions. In the coordination sphere there are two o-phenanthroline molecules bonded as chelates, and two pseudohalide groups linked to the central Cu(II) atom *via* nitrogen atoms. The Cu(II) atom has a distorted octahedral coordination sphere with the –NCX ligands in *cis*-positions.

In electronic absorption spectra we have observed the d–d band at 12900 cm^{-1} for both complexes.

It has been proposed [1, 2] that if the splitting of this band is 5000 cm^{-1} and two peaks are observed with equal intensities, then the complex has a *cis*-octahedral stereochemistry. If, however, the splitting is less than 3000 cm^{-1} and the two peaks occur with different intensities, the compound has a trigonal bipyramidal stereochemistry. Our results support the opinion [6] that the information based on the data from the electronic spectra is not unambiguous in the determination of stereochemistry in compounds with such types of coordination polyhedra. In our case the relevant band is not split and the complex has a *cis*-octahedral stereochemistry.

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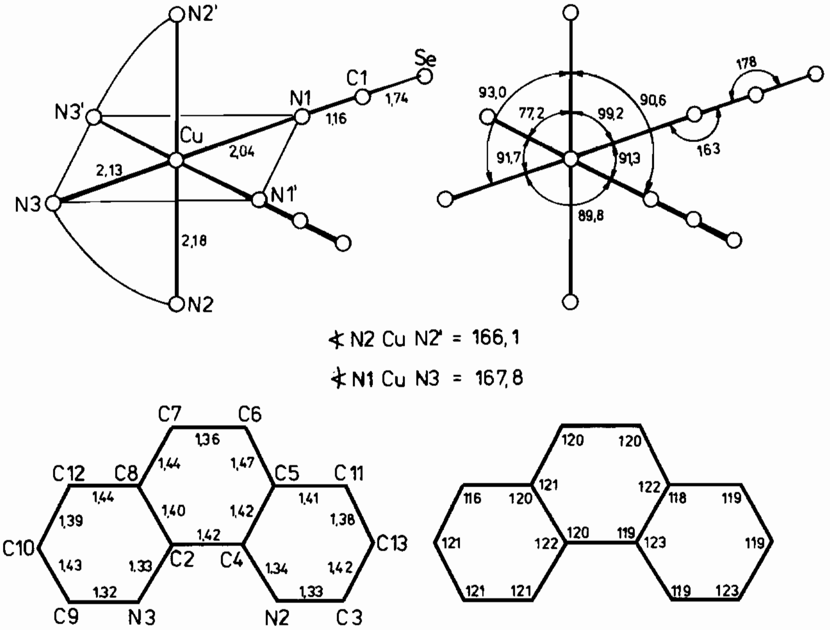

Fig. 1. Stereochemistry, numbering, bond lengths (Å) and angles (°) in the Cu(o-phen)$_2$(NCSe)$_2$ molecules.

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