spectroscopic evidence, that the thiioether sulfur is not coordinated to copper(II), even though there are potentially favorable chelate ring size with sulfur and nitrogen as coordinating atoms. Bridging of the copper centers by carboxylate groups leads to a two-dimensional polymeric structure approach. The isostructural copper(II) complex with its cadmium analogue (F.deMeester,D.-J.Hodgson, J.Am. Chem.Soc. 99,6884 (1977)). The copper(II) atom exhibits a (4+2) tetragonally elongated Cu(NCS)2 coordination octahedron with Cu-O 1.936(6), 1.951(6) Å, Cu-N 2.001(8), 1.995(8) Å, Cu-O axial 2.729(7), 2.703(7) Å. The metrical details for the S-methyl-cysteine ligand show no unusual features. Crystal and refinement data for ZnC6H6O6S4, Sn(Phen)2(NCS)2, Cu(II) phen = phenanthroline and bipy = bipyridine. In co=lection

the differences in the distortion degree of coordination polyhedra. The cations

mainly in bonding angles in equatorial plane while differences in interatomic distances are negligible. In studying the properties of bipyridine complexes we have found that the cation distortion isomerism (Harrison et al. J. Chem. Soc. Dalton (1981) 1556) can also be registered under other experimental conditions as described. Two isomeric forms were prepared for Cu(bipy)2(NCSe)2 (IV and V) which differ in their EPR and IR spectra. We expect that α- and β-isomers will also differ in the distortion degree of their coordination polyhedra which should be intermediates between trigonal bipyramidal and tetragonal pyramidal. The comparison of X-ray results shows that the exchange of neutral ligand causes changes in the configuration of Cu(II) coordination polyhedra and the exchange of pseudohalogenide ligands in this type of complexes causes a different deformation degree at given type of coordination polyhedra.

the dia­compressed coordination polyhedra. The cations

This is the first crystal structure reported of a metal complex of lipoic acid.

09.4-37 STEREOCHEMISTRY OF Cu(II) AND ITS PECULIARITY IN PORPHYRIN ANALOGUES COMPLEXES WITH PHENANTHROLIDINE AND BIPYRIDINE LIGANDS.


In connection with mutual influence of ligands in Cu(II) complexes (Kabešova, uaso, Chem. Zvesti (1983) 34 500) the properties of the following complexes were investigated: [Cu(phen)$_2$(NCS)$_2$] (I), [Cu(phen)$_2$(NCS)$_2$(II) [Cu(bipy)$_2$(NCS)$_2$(II), NCS$_2$ (IV), and Cu(bipy)$_2$(NCS)$_2$(V) where phen = phenanthroline and bipy = bipyridine. For complexes I-IV, their crystal structures were solved (Sedov et al., Koord. Khim.,(1982) § 1062 (I, II), Sedov et al. Enorg. Chem. Acta (1983) 72 73 (III); Sedov et al. Chem. Zvesti (1983) 37 43 (IV). Complexes with phen are isostructural and Cu(II) is pseudo-octahedrally coordinated. An exchange of pseudohalogenide ligands causes the axial distortion of coordination polyhedra. Complexes with bipy in both octahedra have a quasi-trigonal bipyramidal coordination of Cu(II) and in the case of (III) two symmetrically independent coordination polyhedra of Cu(II) were found. Also here, the exchange of pseudohalogenide ligands causes the differences in the distortion degree of coordination polyhedra. The cations

[Cu(bipy)$_2$(NCX)$_2$] where X = S, Se, differ

09.4-38 Conformational Trends in the Metalloporphyrin Series Ni(TMP), Ni(THC), and Ni(THBC). By Paul B. Sweezeon and James A. Ibers, Department of Chemistry, Northwestern University, Evanston, IL 60201, U.S.A.

The isobacteriochlorin macrocycle exhibits an S, ruffled conformation and a bond length pattern indicative of a reduction in aromaticity, both of which are more pronounced than those found in the corresponding porphyrin (Ni(TMP)) and chlorin (Ni(TMBC)). A comparative conformational analysis involving pyramidalization and bond twist angles indicates a significant increase in conformational distortion going from the porphyrin to the chlorin, but only a slight increase in going from the chlorin to the isobacteriochlorin.

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