

P.07.01.1*Acta Cryst.* (2005). A61, C295**Synthesis and Structure of the 1:1 Adducts of Copper (I) Halides with Bis-(benzophenone) Ethylenediimine**

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The steric, electronic, and conformational effects imparted by the coordinated ligands play an important role in modifying the properties of the prepared metal complexes [1].

Reaction of copper (I) halides, CuX, with nitrogen-based ligands yields adducts, CuLX_n. The number of ligands bound to the monovalent copper (I) seems to be influenced greatly by both the chemical nature and geometry of the ligand L and the type of halogen, X, used [2].

1:1 adducts of bis-(benzophenone) ethylenediimine (bz₂en) with CuX (X= Cl, Br, I) [Cu₂X₂(C₅₆H₄₈N₄)], have been synthesized and the structures of the solid complexes established by single-crystal X-ray diffraction. The adducts, surprisingly, are ionic. The chloro and bromo complexes crystallize in the monoclinic crystal system with space group C2/c, but the iodo complex crystallizes in the monoclinic crystal system with space group P2₁/c. The complexes are very stable towards atmospheric oxygen in the solid state.

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Keywords: copper (I) complexes, schiff base, crystal structures

P.07.01.2*Acta Cryst.* (2005). A61, C295**Synthesis and Structural Analysis of a Number of Hexacoordinate Heteroleptic Non-VSEPR Molybdenum and Tungsten Complexes**

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The development of improved models for chemical bonding has always benefited from specific cases in which the existing models fail. One well-known example is the failure of the widely used Valence Shell Electron Pair Repulsion (VSEPR) model. In recent years, many exceptions, represented by "Non-VSEPR" compounds, have been reported. On the basis of ligands similarity these compounds are classified as "homoleptic" and "heteroleptic" systems. Because of their simplicity, homoleptic systems have been studied more than heteroleptic systems. [1], [2] Many quantum chemical calculations on these systems have been reported in the past years. Tungsten and molybdenum complexes have an important role in the extension of non-VSEPR structures and bonding in d⁰ systems.[3] In this research a number of hexacoordinate heteroleptic complexes of molybdenum and tungsten have been synthesized. Indeed, the distortions from the regular octahedron in heteroleptic hexacoordinate d⁰ complexes have played an important historical role in drawing the attention of theoreticians to possible deviations from the usual structures. The structures of these complexes have been characterized by X-ray single crystal diffraction techniques. Experimental data confirm the results of DFT calculations and show good relationship with the Non-VSEPR compounds.

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Keywords: inorganic synthesis, structural analysis, non-VSEPR

P.07.01.3*Acta Cryst.* (2005). A61, C295**Crystal and Molecular Structure of Bis-n-octyl-hydroxy-naphthaldiminato Cu(II). A Study Including Magnetic Properties of Also N-dodecyl and N-octadecyl Derivatives**

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N-R alkyl substituted Schiff bases with R-aliphatic long chains have been used to synthesize a variety of coordination compounds for liquid crystals and Langmuir-Blodgett films applications [1,2].

The present study shows the synthesis and X-ray structure of bis N-octyl-hydroxynaphthaldiminato-copper(II) complex. It crystallizes in the R-9 (#148) space group with a = b = 42.273(25), c = 5.164(3), α = β = 90°, γ = 120°, Z = 9, V = 7992(14) Å³. A total of 2020 reflections with F > 6σ(F) were measured, yielding R (Rw) = 0.052 (0.069) values. The molecular structure shows the copper atom in a planar environment and the octyl chains parallel to each other. The crystal packing shows stacked units intermolecularly separated by 3.61 Å, probably due to π-π electron interactions between naphthyl groups.

Also the N-dodecyl and N-octadecyl derivatives have been obtained and characterized. These three compounds show antiferromagnetic behavior at room temperature while they are normal around 6K. These facts are interpreted in terms of disorder observed in the structures at room temperature.

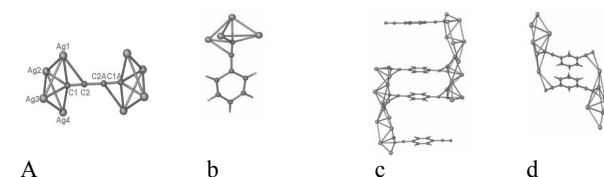
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Keywords: liquid crystals, Schiff-base ligands, antiferromagnetism

P.07.01.4*Acta Cryst.* (2005). A61, C295**Silver Complexes Containing 1,3-Butadienydiide C₄²⁻ and Ar(C≡C)_n (n = 1, 2)**

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Silver 1,3-butadienydiide (Ag₂C₄), a higher homolog of silver(I) acetylenediide (Ag₂C₂), is a light gray amorphous powder (containing ~25 wt% metallic silver) that is explosive when heated (mp 130°C, dec) and sensitive to mechanical shock.^[1] The syntheses and X-ray analyses of a series of double and multiple salts of Ag₂C₄ have shown that the linear C₄²⁻ dianion invariably exhibits a μ₈-ligation mode (Figure a), each terminal being capped by four silver atoms in a butterfly or planar configuration that is consolidated by argentophilic interaction. Similar terminal coordination modes are also found in the double salts of silver phenylacetylenide, Ag(C₆H₅C≡C) (Figure b), and silver *p*- and *m*-phenylenediethynediide, Ag₂(C≡CC₆H₄C≡C) (Figure c and d). These results are consistent with the observation that the highest ligation number^[2] of C₄²⁻ is eight, i.e. four at each end.



[1] Zhao L., Mak T.C.W., *J. Am. Chem. Soc.*, 2004, **126**, 6852-6853. [2] Guo G.-C., Mak T.C.W., *Chem. Commun.*, 1999, 813-814.

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