

Oral Contributions

[MS25 - 05] Charge Density Study of $[\text{Cu}_2(\mu_2\text{-I})_2(2,6\text{-dimethylpyridine})_2]$. Marek Fronc^a, Jozef Kožíšek^a, Lukáš Krivosudský^b, Ján Šimunek^b

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The bonding properties of copper are of great importance for inorganic as well as bio-inorganic chemistry. It is central atom in many metalloproteins (many of them play important role in respiration and activation of the dioxygen, where it exhibits different coordination geometry. Copper(I)-copper(I) interaction attracts the attention of the chemists, because it is related to the binuclear centre of the cytochrome c oxidases and also plays important role in photoluminescence. Copper complexes as the model compounds for the metalloproteins allow to study chemistry of active sites in them. These types of the chemical processes are also important in the development of the new chemical technologies as well as new catalysts based on the metals like copper. $[\text{Cu}_2(\mu_2\text{-I})_2(2,6\text{-dimethylpyridine})_2]$ complex was prepared and its structure determined in 1977 [1] and 1989 [2]. It is colorless, air-sensitive compound. X-ray data collections were performed on an Oxford Diffraction Gemini R four circle diffractometer, using Mo-K α radiation at 100(1) K. Two dataset were collected for the different crystals, because the samples decomposed during the measurement. Data reduction was done by CrysAlis 171.36.24a. Crystal structure was refined by SHELXL program and electron density study and topological analysis were performed by XD program package. Interatomic distance Cu(1)-Cu(2) 2.5471(2) Å is smaller than corresponding sum of the van der Waals radii (2.8 Å) – this suggests possible Cu-Cu interaction. From the Raman spectroscopy was identified

valence vibration of the Cu-Cu (220 cm⁻¹) and it was also supported by theoretical calculations (220.96 cm⁻¹). Topological analyses of the charge density shows for the copper atoms coordination bonds Cu-N and ionic interaction with iodine atoms and possibly also for Cu-Cu interaction. This will be further discussed. This work has been supported by Slovak Grant Agency APVV (APVV-0202-10) and VEGA-1/0679/11.

[1] Campbell J.A., Raston C.L., White A.H.: Aust. J. Chem. 30, 1937 (1977)

[2] Healy P.C., Kildea J.D., Skelton B.W., White A.H.: Aust. J. Chem., 42, 115 (1989)

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