Poster Presentations

[MS13-P01] Charge density study of ternary copper complex

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Many copper complexes with a variety of organic chelating ligands have been shown to possess biological activities. In order to study relationship between these potential biological activities and electronic structure, a good quality crystal of (3,5-dichlorosalicylate)-(2,9-dimethylphenanthroline)-(dimethylsulfoxide) copper complex was prepared. Experimental X-ray data were collected at Oxford Diffraction Gemini R diffractometer equipped with a Ruby CCD detector and a graphite mono-chromator, using Mo-Kα radiation at 100(1) K. Data for multipolar refinement consists of two different experiments using 2.0 and 1.2 kW power supply on X-ray tube as well. Data collection strategy was as follows: 102 (11) runs, 240630 (23151) diffractions, resolution till 0.41 (0.67) Å. Data reduction was done by CrysAlis171.35.19 and an average redundancy of 7.5 (3.1) gives Rint 0.035 (0.039) and R(σ) 0.017 (0.036). Crystal structure was solved and refined by using SHELXS-97 and SHELXL-97. Starting parameters for multiple refinement were taken from a routine SHELXL refinement and all other refinements were carried out on F using the XD suite of programs [1]. The results of the experimental topological analysis of electron density will be discussed.

This work has been supported by Slovak Grant Agency APVV (APVV-0202-10).

[1] P. Coppens, X-ray Charge Densities & Chemical Bonding, Oxford University Press, 1997.

Keywords: charge density; ternary copper complexes; electronic structure