Poster Presentation

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Charge density study of [CuI/II(bite)]+/2+ (bite = biphenyldiimine dithioether) complexes

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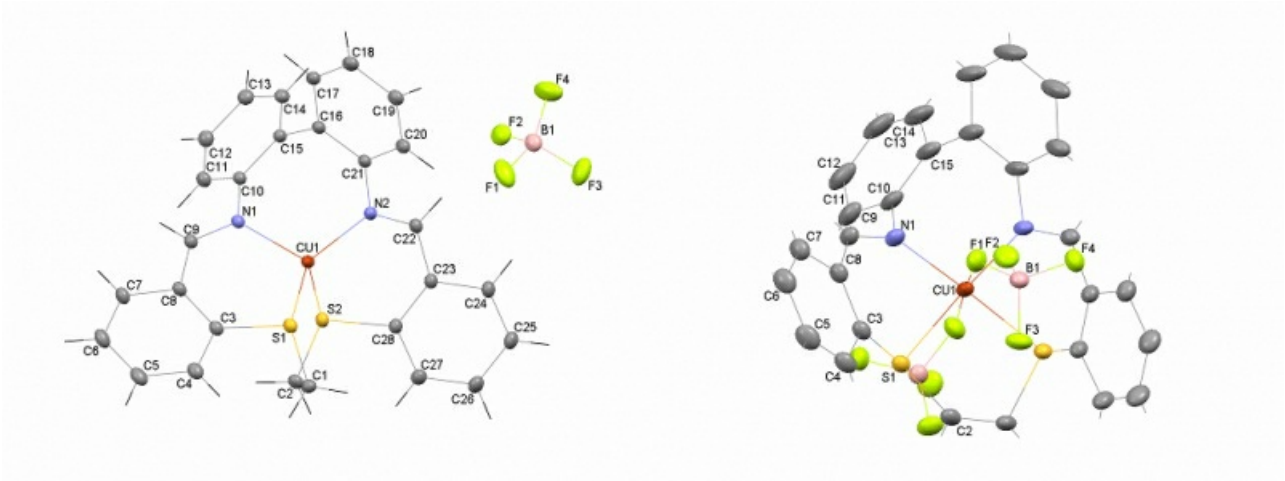
For the presented study two analogous coordination compounds of the copper, [Cu(bite)](BF4) and, [Cu(bite)](BF4)2 (bite = biphenyldiimine dithioether, C28H22N2S2) with copper in oxidation state +I and +II were selected [1]. In the originally work both molecules were synthesized as small-molecule analogue to study properties of the active centre of cuproproteins. In this study we would like to present electron density study of these compounds for the data obtained on a new diffractometer in comparison to the results obtained for the same complexes in the past with the use of Oxford Geminy R diffractometer.
Experiments were performed by means of Stoe STADIVARI diffractometer equipped with a Dectris Pilatus 3R 300K and a Incoatec IμS Ag High Brilliance microfocus source (Ag-Kα, λ = 0.56083 Å) at 100 K using a nitrogen gas open-flow cooler Cobra Oxford Cryosystems. Data reduction was processed using X-Area [2]. Multipole refinement and the topological analysis were performed using XD program package. Electronic structure and the results of AIM analysis will be discussed.
[1] Flanagan, S. et. al. (1997) J. Am. Chem. Soc., 119, 8857-8868.
[2] STOE & Cie GmbH (2016). X-Area 1.76, software package for collecting single-crystal data on STOE area-detector diffractometers, for image processing, scaling reflection intensities and for outlier rejection; Darmstadt, Germany.



Keywords: electron density, copper(I) complex, copper(II) complex