

# CRYSTAL STRUCTURE OF DIMERIC Cu(I) HALIDES $\pi$ -COMPLEXES WITH DISUBSTITUTED DERIVATIVES OF PSEUDOTHIOHYDANTOIN

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Thiazolidinone derivatives possess luminescence and nonlinear-optical (NLO) properties and one of the ways to improve those properties, in particular, is the formation of corresponding coordination compounds. Previously, we have synthesized and determined the crystal structure of a novel copper(I)  $\pi$ -complex  $[\text{Cu}_4(\text{dapt})_2\text{Cl}_4] \cdot 0.38\text{EtOH}$  with diallyl derivative of pseudothiohydantoin (3-allyl-2-(allylimino)-1,3-thiazolidin-4-one) and have studied its photoinduced nonlinear optical properties, namely – laser stimulated second order susceptibility, which achieves a magnitude of 2.2 pm/V.

In the present work, by means of alternating current-electrochemical synthesis four novel Cu(I)  $\pi$ -complexes of  $[\text{Cu}_2(\text{papt})_2\text{Cl}_2]$  (**1**),  $[\text{Cu}_2(\text{papt})_2\text{Br}_2]$  (**2**),  $[\text{Cu}_2(\text{eapt})_2\text{Cl}_2]$  (**3**),  $[\text{Cu}_2(\text{eapt})_2\text{Br}_2]$  (**4**) compositions (*papt* – 2-(phenylimino)-3-allyl-1,3-thiazolidin-4-one, *eapt* – 2-[(2-hydroxyethyl)imino]-3-allyl-1,3-thiazolidin-4-one) were obtained and studied by X-ray single crystal diffraction (Table 1). All compounds crystallize in the monoclinic centrosymmetric space group  $P2_1/n$  and form centrosymmetric dimeric  $[\text{Cu}_2\text{L}_2\text{Hal}_2]$  fragments (Fig. 1). In this fragment both Cu atoms are connected to the bonding halogen atoms, forming central planar  $\{\text{Cu}_2\text{Hal}_2\}$  four-membered ring. Both *papt* or *eapt* molecules in **1-4** are coordinated to the metal centers through their imino N atom and double C=C bond of allyl group acting as bidentate chelate  $\pi, \sigma$ -ligand.

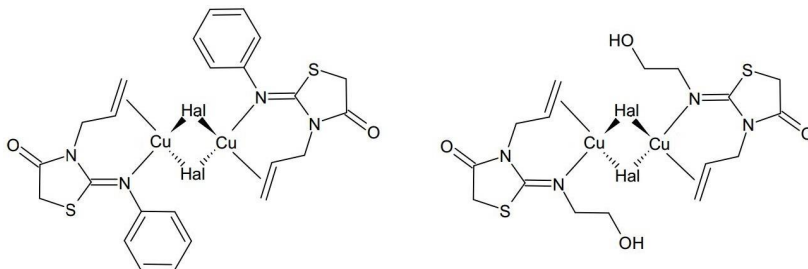


Fig. 1. Centrosymmetric dimeric  $[\text{Cu}_2\text{L}_2\text{Hal}_2]$  fragments in **1-4**, Hal = Cl, Br

Table 1. Selected crystal data of **1-4**

| №        | Composition                               | $V, \text{\AA}^3$ | C=C distance, $\text{\AA}$ |
|----------|---|-------------------|----------------------------|
| <b>1</b> | $[\text{Cu}_2(\text{papt})_2\text{Cl}_2]$ | 1269.9(8)         | 1.363(3)                   |
| <b>2</b> | $[\text{Cu}_2(\text{papt})_2\text{Br}_2]$ | 1295.52(12)       | 1.359(4)                   |
| <b>3</b> | $[\text{Cu}_2(\text{eapt})_2\text{Cl}_2]$ | 1073.0(6)         | 1.364(7)                   |
| <b>4</b> | $[\text{Cu}_2(\text{eapt})_2\text{Br}_2]$ | 1107.1(6)         | 1.374(8)                   |