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Research paper

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ACCEPTED MANUSCRIPT

An unusual diverse coordination of silver(I) with N-allylthiohydantoin ligand in the presence of benzene- and *p*-toluenesulfonate anions

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Highlights:

- Two novel complexes with unusual diverse coordination of Ag(I) with N-allylthiohydantoin were studied
- Different Ag(I) arrangements are determined by variable thiohydantoin coordination modes
- Simulations presence of molecular ligand and its ionic form were observed

Abstract: Crystalline coordination compounds silver(I) $[Ag_{2}(HL)_{4}(C_{6}H_{5}SO_{3})_{2}] \cdot 0.5C_{3}H_{7}OH$ (1) and $[Ag_{2}(HL)(L)(CH_{3}C_{6}H_{4}SO_{3})]$ (2) (HL = 3-(prop-2-en-1-yl)-2-thioxoimidazolidin-4-one) have been obtained using silver(I) salts and the organic ligand HL. Three independent Ag(I) atoms in crystal 1 adopt exclusively different coordination environment: tetragonal pyramidal, seesaw and distorted tetrahedral. In crystal 2 metal ions coordination polyhedra are characterized by seesaw and distorted tetrahedral arrangements. Thiohydantoin molecules in both structures are attached to Ag(I) only through thiohydantoin S-atom, while its anionic form in 2 plays a role of N,S-linker. $C_6H_5SO_3^-$ anions in 1 are bound to the Ag(I) ions in a bridging mode, connecting silver ions into serpentine-like $\{Ag_4(C_6H_5SO_3)_4\}_n$ chains, within which silver ions are additionally bind with μ_2 -S atoms of HL. Simultaneous coordination of HL and L^- moieties in polymeric chains of 2 allow the formation of Ag....Ag metallophilic interactions with the distance range of 2.99 -3.13 Å.

Keywords: silver(I); benzenesulfonate anion; toluenesulfonate anion; thiohydantoin; crystal structure.

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