Poster Presentation

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Experimental charge density studies of silver (I) complex

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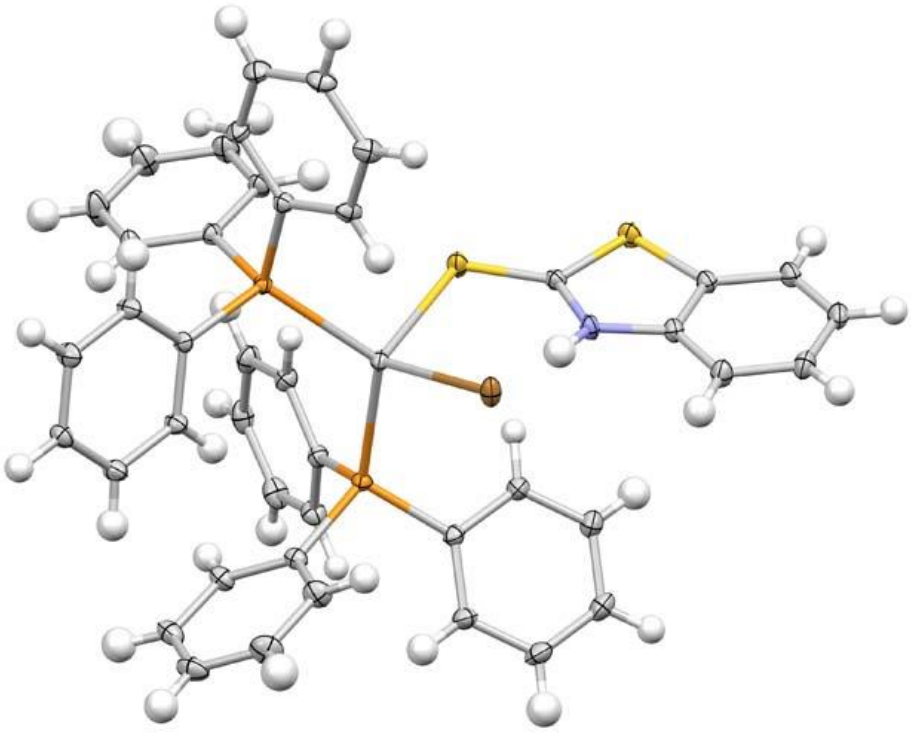
The antimicrobial [1] as well as antitumor activity of silver(I) complexes has been attributed to their interactions with nucleic acids, in the latter case preferentially with the bases rather than the phosphate groups [2]. The ability of silver(I) complexes to adopt structural diverse geometries with variable nuclearities , on the other hand, makes the study of silver(I) chemistry very attractive [1]. In the course of our studies of silver complexes with thioamide ligands we have determined the experimental charge density distribution in new silver(I) bromide complex with 2-mercaptobenzothiazole (mbztH) and triphenylphosphine (tpp) [AgBr(tpp)2(mbztH)], which allowed us to study e.g. the transfer of electron density to the bonding regions and the detailed analysis of different intra- and intermolecular interactions. In view of strong anticancer activity for MCF-7 (IC50 1.75±0.25 μM) [3] of (1) and its sulfur containing ligand, this structure can be very interesting. Moreover the structure of (1) contains two independent complex molecules in asymmetric part of the unit cell, which together with the charge density description of mbztH and tpp allowed us to study different transferability approaches.

[1] *S. Zartilas, S. K. Hadjikakou, N. Hadjiliadis, N. Kourkoumelis, L. Kyros, Maciej Kubicki, M. Baril, I S. Butler, S. Karkabounas, J. Balzarini: Inorganica Chimica Acta 362 (2009) 1003–1010,* ***[2]*** *C.N. Banti, S.K. Hadjikakou, Metallomics, 5, 569-596, (2013),* ***[3]*** *C.N. Banti, A.D. Giannoulis, N. Kourkoumelis, A.M. Owczarzak, M. Kubicki, S.K. Hadjikakou, (2013) submitted for publication*



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