s13.m42.p1 Au•••H-C Interactions in Gold(I) Complexes with Benzyl Imidazolyl Phosphine Ligands. Fiorella Bachechi^a, Alfredo Burini^b, Rossana Galassi^b, Bianca Rosa Pietroni^b, ^aIstituto di Cristallografia, C.N.R., Area della Ricerca di Roma, C.P. 10, I-00016 Monterotondo St. (Roma), Italy, and ^bDipartimento di Scienze Chimiche, Universita di Camerino, Via S.Agostino 1, I-62032 Camerino, Italy. E-mail: fiorella.bachechi@ic.cnr.it

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Secondary interactions in gold(I) compounds have assumed considerable interest, since they have a profound influence on chemical and physics properties, structures and conformations of gold complexes. In the last years a large number of secondary bonding interactions has been discovered in compounds of gold(I), mostly of the general type L-Au-X, where L is a phosphine ligand and X is a halide or a pseudohalide. Distinct kinds of interaction involving gold atoms are: Au•••Au (aurophilic interaction), Au•••X where X is a halide, Au••• π -system, Au•••H-C. This last type of contact is very rare either as hydrogen bond or as agostic interaction. The tertiary phosphines (BzIm)Ph₂P, 1-benzyl-2-imidazolyl diphenyl phosphine, and (BzIm)₃P, tris-(1-benzyl-2-imidazolyl)phosphine, have features to systematically allow Au•••H-C contacts, also coexisting with aurophilic interactions. In fact, they are able to bring the hydrogen atoms of the benzyl groups in close position to the gold atom by a change of conformation. In the complex [(BzIm)Ph₂PAuCl] [1], where only one benzyl imidazolyl group is present, the assumed conformation is favourable for the CH₂ group to have one hydrogen atom at close distance from Au (2.62 Å). In the complex, [(BzIm)₃PAuCl], two benzyl imidazolyl groups position one hydrogen atom of each CH₂ group at close distances from gold (2.83 and 2.95 Å). In the tetranuclear gold cluster $[\{(BzIm)_3P\}_2Au_4Cl_2]^{2+}$ with the two (BzIm)₃P phosphines, which act as bihapto ligands, two gold atoms each interact with one hydrogen atom at distances of 2.57 and 2.59 Å.

 Burini, A.; Pietroni, B. R.; Galassi, R; Valle, G.; Calogero, S. Inorg. Chim. Acta 1995, 229, 299-305. **s13.m42.p2 1:1 Complex of N-methylmorpholine Betaine with Salicylic Acid.** <u>E. Bartoszak-Adamska</u> and M. Jaskólski, Department of Crystallography, Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland. E-mail: ela@amu.edu.pl

Keywords: N-methylmorpholine betaine; Salicylic acid; Hydrogen bonds

Salicylic acid is a commonly used anionic drug component, e.g. with benzylamine, chloroquine, choline, quinine, morpholine, picolamine, etc. because of its own pharmacological and biological activity (analgesic, antipyretic, antiinflammatory activity). N-Methylmorpholine betaine (MMB) and salicylic acid (SAL) form a 1:1 complex, in which the acidic proton is transferred from the acid to the betaine zwitterion. The crystals are orthorhombic, space group Pbca, with a=9.4702(6), b=13.0559(7) and c=45.226(2) Å (at 140 K). The asymmetric unit is comprised of two MMB⁺·SAL⁻ units (A and **B**), each formed by a short O-H…O hydrogen bond (2.542(2) and 2.474(2) Å) between the carboxylic group of the betaine cation and the carboxylate group of the anion. The morpholine rings (A and B) are in the chair conformation with the CH₂COOH group in the equatorial and the methyl group in axial positions. The hydrogen atoms of the COOH groups of the MMB⁺ cations are situated at oxygen atoms which are anti to the betaine nitrogen atoms. The salicylate anion in both complexes is stabilized by a short intramolecular O-H...O hydrogen bond, which is shorter in complex A (2.472(2) Å). The donors in those intramolecular interactions are the phenolic OH groups, which are not involved in any other hydrogen bonds. An important difference between the two cation ... anion units is that in complex B the two O-H...O bonds are accepted by one carboxylate oxygen atom of the salicylate anion, while in complex A the inter- and intramolecular O-H...O bonds are accepted by different salicylate O atoms. The relatively high density of the crystals ($D_x = 1.413 \text{g/cm}^3$), which consist of atoms not heavier than O, is a consequence of (i) the electrostatic attraction between the MMB⁺ cations and the SAL⁻ anions, (ii) the strong intermolecular O…O hydrogen bonds between the MMB+ cations and the SAL⁻ anions, and (iii) the numerous C-H…O interactions. The crystal packing is dominated by helical arrangement of the structural components. This is manifested as a "cross pattern" visible in the diffraction data.