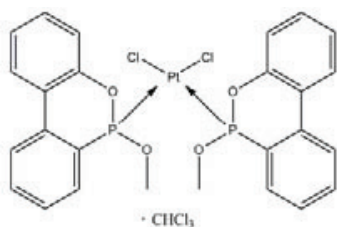


FA4-MS04-P08

Molecular Association in the Dichloridobis(2-methoxydibenzo[c,e]-[1,2]oxaphosphorine-κ-P) platinum(II): Trichloromethane 1:1 Solvate. Tamas Holczbauer^a, Csaba Németh^b, Éva Pfeifer^b, János Mink^b, Andrea Kerényi^c, György Keglevich^c, Mátyás Czugler^a. ^a*Hung. Acad. Sci., Chemical Research Center, Structural Chemistry*. ^b*X-ray Diffraction*, and ^c*Department of Molecular Spectroscopy, University of Technology and Economics, Department of Organic Chemistry and Technology, Budapest, Hungary*.
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The X-ray structure determination of the oxaphosphorine-platinum-dichloride complex showed that it crystallized with one chloroform solvent molecule. The solvent molecules are stuck in channels made up by the complex molecules. These open solvent tubes are parallel to the crystallographic a axis and penetrate the macroscopic crystals throughout. Each chloroform molecule connects to its complex molecule via a pronounced C-H ... O bond. The chloroform molecules are clearly disordered. To decide the dynamic or static nature of disorder X-ray diffraction data were collected at low and at room temperatures, too. IR and Raman spectroscopy were also used to determine the binding angles and the intermolecular C-H ... O bonds' characteristics. The understanding of the role of the chloroform molecule in the solid phase is important for the structure and stability of the crystal. As a first step we reported the LT crystal structure of the title associate [1]. RT structure and spectroscopic results will be compared and analyzed in light of a possible disorder model.



Scheme of the asymmetric unit of the crystal

[1] Holczbauer, T., Keglevich, Gy, Kerényi, A., Czugler, M., *Acta Crystallogr.*, **2009**, E65; m347-m348.

Keywords: inclusion complex; molecular channel; disorder

FA4-MS04-P09

Structural Investigations of Cd Complexes of Bisphosphonate Ester Derivatives. Jonna Jokiniemi^a, Jouko J. Vepsäläinen^b, Harri Nätkinniemi^a, Sirpa Peräniemi^b, Markku Ahlgrén^a. ^a*Department of Chemistry, University of Joensuu, P.O.Box 111, 80101, Joensuu, Finland*. ^b*Laboratory of Chemistry, Department of Biosciences, University of Kuopio, P.O. Box 1627, 70211, Kuopio, Finland*.
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Bisphosphonic acids have attracted close attention because of their utility in supramolecular chemistry and crystal engineering [1,2]. Usually, the metal bisphosphonates form polymeric materials and microporous solids, with properties that offer a diversity of practical applications in catalysis, ion-exchange and sorption [2-4]. Hydrogen bonds are predominant in these architectures, producing one-, two- and three-dimensional networks. In our continuing research for bisphosphonate ester derivatives, we have prepared three new Cd complexes of (dichloromethylene) bisphosphonic acid P,P-diphenyl, monophenyl and monoethyl ester derivatives. The structures of these compounds were characterized by single crystal X-ray diffraction. All three compounds show a different layered structure. The Cd complex of monophenyl ester derivative consists of 1-D chains with four independent octahedral Cd atoms joined by two bisphosphonate ligands. The chains are connected into layers by phosphonate O atoms, and the adjacent layers are held together by weak π - π stacking interactions. The Cd complex of diphenyl ester derivatives shows a new type of layered structure for metal bisphosphonates, where the bisphosphonate ligand coordinates tridentately to three Cd²⁺ ions. Each CdO₆ octahedron is connected to three CPO₃ tetrahedra and each tetrahedron to three octahedra leading to a 2-D framework consisting of 12-membered cyclic cores. In Cd compound of monoethyl ester derivative, the asymmetric unit contains two independent Cd²⁺ cations connected by bisphosphonate ligands, to form a Cd-bisphosphonate layer. The layers are further interconnected into a 3-D supramolecular network by extensive hydrogen bonds.

[1] A. Clearfield, C.V. Krishnamohan Sharma, B. Zhang, *Chem. Mater.*, **2001**, 13, 3099. [2] R. Fu, S. Hu, X. Wu, *Cryst. Growth Des.*, **2007**, 7, 1134. [3] A. Clearfield, *Progress in Inorganic Chemistry: Metal Phosphonate Chemistry*, ed. K. D. Karlin, Wiley, New York, **1998**, vol 47, pp. 371-510 and references therein. [4] Maeda, K. *Microporous Mesoporous Mater.*, **2004**, 73, 47 and reference therein.

Keywords: bisphosphonates; coordination complexes; single crystal X-ray analysis

FA4-MS04-P10

Supramolecular Chemistry of Reinecke Salt Derivatives. Mátyás Czugler^a, Veronika Kudar^a. ^a*X-ray Diffraction, Structural Chemistry, Chemical Research Center, Budapest, Hungary*.
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One of the oldest complex anion salts, used for long in the analytical chemistry of mainly foodstuffs and of inorganic chemistry is the Reinecke salt, conceived in the 1860s. Apart from early attempts no systematic structural studies were reported for this long-known substance, however. Crystallization of such compounds poses formidable problems as the title salt generally forms rather awkward precipitates. Nevertheless, series of complexes of derivatives of the parent compound were prepared in our laboratory and about half a dozen structure determinations by single crystal X-ray diffraction followed these experiments.