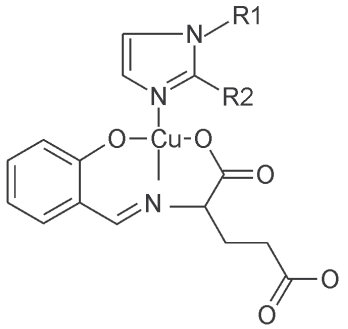
s13.m35.p12 **Structural Aspects of Some Cu(II) Complexes Containing Schiff Base.** Dalma Gyepesová[a], Vratislav Langer[b], Eva Scholtzová[a], Mária Kohútová[c] and Aladár Valent[c], [a]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, SK-845 36 Bratislava, Slovak Republic,* [b]*Department of Environmental Inorganic Chemistry, Chalmers University of Technology, SE-412 96 Göteborg, Sweden and* [c]*Department of Chemical Theory of Drugs, Faculty of Pharmacy, Comenius University, SK-832 32 Bratislava, Slovak Republic. E-mail: uachgyep@savba.sk*

Keywords: Cu(II) complex; Schiff base; B3LYP

A group of copper(II) complexes containing Schiff bases, derived from salicylaldehyde and various amino acids, is interesting due to their biological activities. Structures of (N-salicylidene-*rac*-glutamato)(1-methylimidazole)Cu(II) **I** [1], (N-salicylidene-rac-glutamato)(2-methylimidazole)Cu(II) II [2] and (N-salicylidene-L-glutamato)(2-ethylimidazole)Cu(II) **III** [3] have been determined. Electron structure of these compounds has been investigated by the B3LYP method.



I: R1=CH_3, R2=H
II: R1=H, R2= CH_3
III: R1=H, R2=CH_2CH_3

In the all here presented complexes three donor atoms (O, N and O) of the Schiff base and a fourth donor atom from the imidazole ligand (N) define the basal plane of Cu(II). Depending on different substituents R1 and R2 on the imidazole ring, changes of coordination sphere of Cu(II) is varying (square-planar or square-pyramidal) as well as way of packing of molecules in the crystal. The more detailed discussion will be presented.

[1] Langer, V., Scholtzová, E., Gyepesová, D., Kohútová, M..& Valent, A. (2003). *Acta Cryst.* E**59**, m1181-m1183
[2] Langer, V., Scholtzová, E., Gyepesová, D., Kohútová, M..& Valent, A. (2004). *Acta Cryst.* E**60**, m129-m132
[3] Langer, V., Scholtzová, E., Gyepesová, D., Kohútová, M..& Valent, A.-in preparation

s13.m35.p13 **Molecular Complex Formation of Various Cationic Surfactants with Perfumes and the Stability of the Complexes.** Nahoko Iimura[a] and Yuji Ohashi[b], [a]*Niigata University of Pharmacy and Applied Life Sciences,* [b]*Tokyo Institute of Technology, Japan. E-mail: iimura@niigata-pharm.ac.jp*

Keyword: Surfactant molecular complex; X-Ray analysis; Perfume

Quaternary ammonium cationic surfactants, such as hexadecyltrimethylammonium bromide (C16TAB) make complexes with aromatic compounds (additives) such as phenolic derivatives and basic substances containing drugs from an aqueous, alcohol or acetone solution at low temperatures (<10 C°). The structures of the complex crystals have been analyzed by X-rays. They were very similar to each other [1].

In this work, some perfumes such as guaiacol and 2-methylindole were selected as additives and their complex crystals with cationic surfactants were analyzed by X-rays. The crystal structures have similar features to those of the complexes composed of quaternary ammonium surfactants and aromatic compounds determined so far. (Fig.1) The thermal stability of the complexes was analyzed by thermogravimetry. (Fig.2) It is clear that the volatilization of the perfume molecule was reduced in the complex formation. The thermal stability is closely related to the alkyl chain lengths of cationic surfactants.

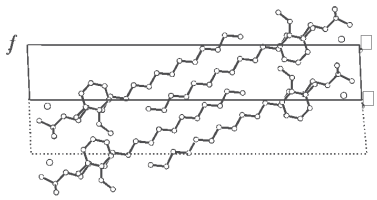


Fig.1 Crystal structure of C16TAB/guaiacol

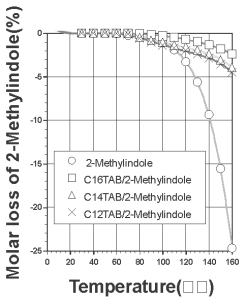


Fig.2 Molar loss of 2-methylindole with temperature in the complex crystals with C16TAB, C14TAB, and C12TAB compared with the pure crystal of 2-methylindole.

[1] Sawada K., Kitamura T., Ohashi Y., Iimura N., and Hirata H., *Bull. Chem. Soc. Jpn*., **71**, 2109-2118 (1998)