

s13.m35.p32 **New Polar Crystal of the Pyridinium Betaine Salt.** Lukasz Wojtas, Katarzyna Stadnicka, Faculty of Chemistry, Jagiellonian University, Ingardena 3, 30-660 Krakow, Poland. E-mail: wojtas@chemia.uj.edu.pl

**Keywords: Pyridinium salts; Phenylphosphinic acid; Polar structure**

In due course of designing structures with pyridinium betaine dye introduced as NLO chromophore, crystals of the salt formed by 1-(4-hydroxyphenyl)-2,4,6-triphenyl-pyridinium cation with phenylphosphinic acid were obtained. The pyridinium betaine shows a large negative solvatochromic effect [1-2] and the main aim of our work was to introduce the molecule into an acid framework to obtain polar crystals suitable for nonlinear optics.

Colourless crystals were obtained by slow evaporation from ethanol solution of the betaine dye and phenylphosphinic acid in molar ratio 1:4. The structure shows polar symmetry (space group Pna2<sub>1</sub>) with a = 29.4720(1) Å, b = 10.3800(3) Å, c = 22.9960(5) Å, V = 7034.92 Å<sup>3</sup>, D<sub>x</sub> = 1.291 Mg/m<sup>3</sup>, Z = 4 and chemical formula 2[C<sub>29</sub>H<sub>22</sub>NO]<sup>+</sup>·2[C<sub>6</sub>H<sub>6</sub>PO<sub>2</sub>]<sup>-</sup>·2[C<sub>6</sub>H<sub>7</sub>PO<sub>2</sub>]. Direct methods was used to solve the structure and refinement by full matrix least-squares on F<sup>2</sup> was converged at R<sub>1</sub> = 0.070, wR<sub>2</sub> = 0.183, S = 1.002 for 7037 unique reflections with Fo > 4σ(Fo).

Presented crystal structure is interesting because it lacks the crystallographic inversion centre which is not typical for salts of such a type. The crystals are built of two kind of alternate layers. The pyridinium betaine layers, in which cation dipoles show an antiparallel arrangement, are separated by the layers consist of anions and acid molecules. It seems that the structure polarity arises from different interactions of upper and lower surfaces of pyridinium betaine layer with adjacent phenylphosphinic layers.

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s13.m35.p33 **Double Complex Salts [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>][M(NO<sub>2</sub>)<sub>4</sub>] (M=Pt or Pd).** Kirill Yusenko, Iraida Baidina, Sergey Korenev, Nikolaev Institute of Inorganic Chemistry, Russian Academy of Science, Siberian Branch, Akademichskay, 2/a, Novosibirsk, Russia. E-mail: yusenko@che.nsk.su

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The structure of [M(NO<sub>2</sub>)<sub>4</sub>]<sup>2-</sup> anions depends on their environment [1]. In this connection it was interesting to prepare salts with the [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>]<sup>2+</sup> cation.

The double complex compounds [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>][Pt(NO<sub>2</sub>)<sub>4</sub>]·1.5H<sub>2</sub>O (I) and [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>][Pd(NO<sub>2</sub>)<sub>4</sub>] (II) are precipitated when water solution of [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>]Cl<sub>2</sub> and K<sub>2</sub>[M(NO<sub>2</sub>)<sub>4</sub>] (M= Pt or Pd) are mixed. Yield is 75-85 %. The complexes are studied by X-ray structure analysis, IR-spectroscopy and DTA. Crystallographic data for **I**: a=7.7583(8) Å, b=9.6385(9) Å, c=10.9641(11) Å, α=97.216(2)°, β=92.090(2)°, γ=112.2500(10)°, P-1, V=749.66 Å<sup>3</sup>, Z=2, d<sub>x</sub>=2.602 g/cm<sup>3</sup>, d<sub>m</sub>=2.70±0.02 g/cm<sup>3</sup>, R=0.0180; for **II**: a=8.0209(8) Å, b=22.167(2) Å, c=7.8453(8) Å, β=98.836(2)°, Cc, V=1378.3(2) Å<sup>3</sup>, Z=4, d<sub>x</sub>=2.316 g/cm<sup>3</sup>, d<sub>m</sub>=2.29±0.02 g/cm<sup>3</sup>, R=0.0247.

The structures are composed of the complex ions [Co(NH<sub>3</sub>)<sub>5</sub>NO<sub>2</sub>]<sup>2+</sup> and [M(NO<sub>2</sub>)<sub>4</sub>]<sup>2-</sup>. In structure I there are molecules of crystallization water. In the structures, the complex ions are bound by the hydrogen bonds along with electrostatic forces. A feature of the crystal structures of the salts is the presence of the pairs of the connected anions (see figure). The O(NO<sub>2</sub>)...Pd distances are 3.003 and 3.184 Å. In structure II, such pairs form the chains. In structure I, the same pairs are isolated. The N(NH<sub>3</sub>)...Pt distance is 3.655 Å. Thus, the coordination Pt and Pd polyhedra are supplemented up to distorted octahedra.

This work presents an analysis of the structure of [M(NO<sub>2</sub>)<sub>4</sub>]<sup>2-</sup> anions and general packing motifs.

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