

s13.m35.p14 **Intramolecular Hydrogen Bonding and Tautomerism in 1-[(2-hydroxy phenylamino) methylene]-2-(1H)-5-phenylazo salicylaldehyde.** Reza Kia^a, Ahmadreza Esmailbeig^a and Sybolt Harkema^b. ^aChemistry Department, Shiraz University, Shiraz, 71454, Iran. ^bLow Temperature Division, Faculty of Science and Technology and MESA+ Research Institute, University of Twente, PO Box 217, 7500 AE Enschede, The Netherlands. E-mail: rkia@chem.ui.ac.ir

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Schiff bases have often been used as chelating ligands in the field of coordination chemistry for obtaining thermotropic liquid crystalline polymers and their metal complexes have been used as radiopharmaceutical for cancer targeting, as model system for biological macromolecule [1]. The tautomerism in the Schiff base ligands plays an important role for distinguishing their photochromic [2] and thermochromic [3] characteristics. Consequently, it is evident that a closely related phenomenon of interest is the possibility of tautomeric isomerism in ortho-hydroxy Schiff bases. Therefore, the structures of this kind of Schiff bases are relevant due to the possibility of finding them in the solid state and/or in solution as keto-amine or phenol-imine tautomers, and their connections with photochromism and thermochromism. In the solid state, salicylaldehyde Schiff bases tend to form (N...H-O) or (N-H...O) types of hydrogen bonding, respectively [4]. In many cases in solution, both types of hydrogen bonds have been observed indicating phenol-imine, O-H...N, keto-amine, O...H-N tautomerism [5]. For the title compound the tautomeric keto-amine isomer is observed with N-H distances of 0.97(3) Å. Strong intramolecular hydrogen bonds are found between the N17 and O15 atoms with an O...H distance of 1.86(2) Å, while the N17...O15 distance is 2.591(2) Å. The value for the N17-H...O15 angle is 135(2)°. An important intramolecular interaction is the O24-H24...O15' hydrogen bond (O24-H15 1.05(2) Å, H24...O15' 1.51(2) Å, angle 172(2)°. Bond lengths in the fragment N17-C16-C11-C12 suggest electronic delocalization. The molecule consists of two almost planar moieties (plane 1 (atoms C1..C6), max. deviation 0.098 Å; plane 2 (atoms C18..C23), max. deviation 0.0010 Å; the interplanar angle being 21.9°.

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s13.m35.p15 **Rietveld Structure Refinement of [Pt(NH₃)₄][ReCl₆].** Ilya Korolkov^a, Alexander Tyutyunnik^b, Sergey Gromilov^a, ^aNikolayev Institute of Inorganic Chemistry, Novosibirsk, Russia, ^bInstitute of Solid State Chemistry, Ekaterinburg, Russia. E-mail: kiv@mail333.com

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Structure of double complex salt [Pt(NH₃)₄][ReCl₆] was refined. Such complexes, obtained by method described in [1], are used to produce solid solutions of platinum metals by their thermolysis. This process is carried out at about 500 - 700 °C. Knowledge about a structure of the complex will help to understand the process. An X-ray powder diffraction pattern of the sample for the structure refinement was collected with a STOE STADI-P diffractometer (Bragg-Brentano geometry, CuKα-radiation, secondary beam monochromator, scintillation counter, 2.0 - 120.0 ° 2θ range, step size 0.02° 2θ, 45 sec counting time per step).

The investigated complex is isostructural to [Pd(NH₃)₄][IrCl₆] [1]. Crystallographic data of [Pt(NH₃)₄][ReCl₆]: a = 11.6164(2) Å, b = 10.9976(2) Å, c = 10.3765(2) Å, V = 1325.69 Å³, space group Cmca, Z = 4, D_x = 3.317 g/cm³. The structure of the complex was refined by GSAS program [2] up to the value of R_p = 5.47% and wR_p = 9.95%. We used the pseudo-Voigt description of the profile. GU, GV, GW, LX and asymmetry were refined. The structure of [Pt(NH₃)₄][ReCl₆] is built of planar ions [Pt(NH₃)₄]²⁺ and distorted octahedra [ReCl₆]²⁻. The symmetry of the both units is 2/m. Since Pt and Re atoms are in the general position, only the positions of chlorine atoms were refined. We have remained the N position unchanged. Average Re - Cl and Pt - N distances are 2.35 Å, 2.05 Å, respectively; valence Cl1 - Re - Cl and N - Pt - N angles are 90.03° and 89.48°, respectively. These data correlate well with the distances and angles for [Pt(NH₃)₄]²⁺ in [Pt(NH₃)₄][PtCl₄] [3] and [ReCl₆]²⁻ in (NH₃)₂ReCl₆ [4] structures known before.

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