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The polymeric anhydrous rubidium hydrogen oxalate

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The anhydrous complex of the rubidium hydrogen oxalate has been synthesized as single crystal and characterized by X-ray diffraction, IR spectroscopy and thermogravimetric study. The structure has been determined from data collected on a Kappa CCD diffractometer and shows the compound to be isostructural with the potassium hydrogen oxalate [1]: it crystallizes in space group $P2_1/c$ ($Z=4$) with the cell parameters $a=4.2940(3)$, $b=13.6230(10)$, $c=7.6689(5)$ and $\beta=101.50(50)^\circ$, slightly different from those found by Hendricks [2]. The structure consists of layers formed by chains of one-edge-sharing rubidium polyhedra, running along the [001] direction and alternating layers of hydrogen oxalate groups, Hox, which are hydrogen bonded. The rubidium atom is sevenfold coordinated with two bridged-chelating Hox ligands and three bridged monodentate hydrogen oxalate.

As expected, the anion group is non planar and is found to be twisted about the C-C bond with an angle of about 15° . It is due to the strong hydrogen bond which is usual in acid salt alkali metal and hydrogen-carboxylates complexes [1][3][4][5]. This hydrogen bond O-H...O' which connects the hydrogen oxalate ions is asymmetric (O-H and H...O' distances are respectively 0.99 and 1.547 Å) and approximately linear (the O-H...O' angle is 176°).

The IR spectrum shows the bands due to the free carbonyl absorption and to oxalate salts as the bands of O-H stretching modes and the thermal decomposition agrees with the XR and IR investigations.

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Structural class distribution for *cis/trans*-PtX₂L₂, X=halogen, L=neutral ligand; the structures of two polymorphs of *cis*-PtCl₂(Bz₂S)₂

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The structural class concept [1] carries information about point group symmetry and may thus be used to answer the question: What point group symmetry is retained in the solid state? Such common features will be of most interest for molecules that have similar crystallochemical nature, like *cis/trans*-PtX₂L₂; X = halogen, L = neutral ligand. *trans*-PtX₂L₂ may adopt point groups C₁, C_s, C₂, C_{2v}, C_i and C_{2h}, while *cis*-PtX₂L₂ is constrained to C₁, C_s, C₂ and C_{2v}. The most frequently observed molecular point group for complexes *trans*-PtX₂L₂ is C_i (78%) followed by C₁ (16%) [2]. Even if *cis*-PtX₂L₂ cannot adopt to C_i it often forms a centrosymmetric dimeric packing arrangement in the solid state. The dimers as observed in the Cambridge Structural Database (2005 release) [3] are classified according to the interaction across the centre of symmetry formed by two i) Pt---X, ii) Pt---L (donor atom), iii) Pt---L (hydrogen atom) and iv) Pt---L (other type) interactions. In many cases the interaction between the complexes forming dimers seems to be small, but in some cases it is of chemical significance. Two polymorphs of *cis*-PtCl₂(Bz₂S)₂ crystallizing in P-1 and C2/c, respectively, have been synthesized. The polymorph in C2/c is more close-packed ($D_x=1.67 \text{ g/cm}^3$) than the one in P-1 ($D_x=1.61 \text{ g/cm}^3$) in conflict with Kitaigorodsky's division of space groups into closest-packed, limiting close-packed, permissible and impossible [4], where P-1 belongs to closest-packed and C2/c permissible. However, it is in agreement with Wilson's idea [5], that by introducing centrosymmetric dimers in the packing description, C2/c is moved from permissible to closest-packed. Structural class frequencies for *cis*-PtX₂L₂ as observed in CSD will be reported and discussed.

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