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Preparation and Molecular Structure of Diaquabis(2,6-dihydroxybenzoato)dioxouranium(VI) Octahydrate

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Metal complexes formed by dihydroxybenzoic acids could be of help in elucidating the metal binding properties of humic-like substances,. which are of major importance in the environmental behavior of metals. In this connection, compounds obtained by reaction of 2,6-dihydroxybenzoic acid with some divalent metal ions have been isolated and fully characterised [1, 2]. Interestingly, the role of hydrogen bonding in favouring the formation of outer-sphere arrangements in the solid state has been shown by X-ray analysis.

Here we report preliminary structural data for the title compound which was obtained by reaction of 2,6-dihydroxybenzoic acid with uranyl acetate in aqueous solution.

Crystal data: monoclinic, space group $C2/m$, $a = 6.704(3)$, $b = 20.171(6)$, $c = 9.454(4)$ Å, $\beta = 99.57(3)°$, $V = 1260.6$ Å^3, $D_c = 1.99$ g cm^{-3}, $D_m = 2.03$ g cm^{-3}, $Z = 2$, MoKα radiation, $\lambda = 0.7107$ Å. 1627 independent reflections were used for the structure determination and refinement (usual $R = 0.033$).

A view of the complex is reported in Fig. 1, together with the more significant bond distances and angles. The molecule consists of uranyl groups equatorially surrounded by two *trans* bidentate carboxylate groups and two oxygen atoms from water molecules. The remaining eight water molecules are hydrogen bonded to the rest of the structure to give intermolecular contacts between neighbouring units.

Also in this case, hydrogen bonding appears to be responsible for uncommon structural features of the complex. In fact, coordination of dioxouranium(VI) by only two carboxylate groups is rather unusual [3] and is probably accounted for by the favourable involvement of an extended network of hydrogen bonds.

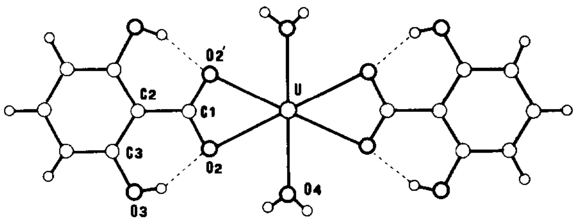

Fig. 1. View of the molecule along the O–U–O axis. The oxygen atoms of the uranyl group, O(1) and O(1)', are not shown. Important bond lengths and angles: U–O(1) 1.760 (0.006), U–O(2) 2.485 (0.003), U–O(4) 2.462 (0.006), C(1)–O(2) 1.275 (0.005), C(3)–O(3) 1.361 (0.006) Å; O(2)–U–O(2)' 51.8 (0.2), O(2)–C(1)–O(2)' 116.6 (0.7) deg.

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Structures and Reactivities of Copper(I) and Silver(I) Complexes of Potentially Quadridentate N_4 and N_2S_2 Donor Ligands

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In designing model complexes for the active sites in copper proteins it is important to know the influence of different hetero-atoms and conformational changes of the carbon skeleton on the chemical and physical properties of the metal centre.

We have investigated the structural properties of copper(I) and silver(I) complexes with potentially quadridentate N_4 and N_2S_2 donor ligand systems, schematically represented in Fig. 1, which have the connecting (*R*)(*S*)-1,2-diiminocyclohexane group in common.

From the reaction of the N_4 donor ligand with $M(O_3SCF_3)$ ($M = Cu^I$ or Ag^I) we obtained dimeric