

Dihydroxyacetone phosphate, DHAP, in the crystalline state: monomeric and dimeric forms.

Autorzy

Katarzyna Ślepokura

Tadeusz Lis

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It was shown that dihydroxyacetone phosphate may exist in both monomeric DHAP ($C_3H_7O_6P$) and dimeric DHAP-dimer ($C_6H_{14}O_{12}P_2$) form. Monomeric DHAP was obtained in the form of four crystalline salts: $CaCl(DHAP) \cdot 2.9H_2O$ (**7a**), $Ca_2Cl_3(DHAP) \cdot 5H_2O$ (**7b**), $CaCl(DHAP) \cdot 2H_2O$ (**7c**), and $CaBr(DHAP) \cdot 5H_2O$ (**7d**) by crystallization from aqueous solutions containing DHAP acid and $CaCl_2$ or $CaBr_2$, or by direct crystallization from a solution containing DHAP precursor and $CaCl_2$. At least one of the salts is stable and may be stored in the crystalline state at room temperature for several months. The dimeric form was obtained by slow saturation of free DHAP syrup with ammonia at $-18\text{ }^\circ\text{C}$ and isolated in the form of its hydrated diammonium salt $(NH_4)_2(DHAP\text{-}dimer) \cdot 4H_2O$ (**8**). The synthesis of the compounds, their crystallization, and crystal structures determined by X-ray crystallography are described. In all **7a–d** monomeric DHAP exists in the monoanionic form in an extended (in-plane) cisoid conformation, with both hydroxyl and ester oxygen atoms being synperiplanar to the carbonyl O atom. The crucial structural feature is the coordination manner, in which the terminal phosphate oxygen atoms act as chelating as well as bridging atoms for the calcium cations. Additionally, the DHAP monoanions chelate another Ca^{2+} by the α -hydroxycarbonyl moiety, in a manner observed previously in dihydroxyacetone (DHA) calcium chloride complexes. In dimeric **8** the anion is a trans isomer with the dioxane ring in a chair conformation with the hydroxyl groups in axial positions and the phosphomethyl group in an equatorial position.

Słowa kluczowe

Dihydroxyacetone phosphate, DHAP, DHAP-dimer, DHAP synthesis, Stable DHAP salts, X-ray crystal structure

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