

Crystal structures of dihydroxyacetone and its derivatives.

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Streszczenie

The crystal and molecular structures of three crystalline forms of the dihydroxyacetone dimer, $C_6H_{12}O_6$, DHA-dimer: α (**1a**), β (**1b**), and γ (**1c**), the hydrated calcium chloride complex of dihydroxyacetone monomer, $CaCl_2(C_3H_6O_3)_2 \cdot H_2O$, $CaCl_2(DHA)_2 \cdot H_2O$ (**2a**), the tetrahydrated calcium chloride complex of dihydroxyacetone monomer, $CaCl_2(C_3H_6O_3) \cdot 4H_2O$, $CaCl_2(DHA) \cdot 4H_2O$ (**2b**), the dihydroxyacetone monomer, $C_3H_6O_3$, DHA (**2c**), and dihydroxyacetone dimethyl acetal, $C_5H_{12}O_4$, $(MeO)_2DHA$ (**3**) are described. Compounds **1a** and **2b** crystallize in the triclinic system, and **1b,c**, **2a,c**, and **3** are monoclinic. Molecules of all forms of dihydroxyacetone dimer **1a,b**, and **1c** are the *trans* isomers, with the 1,4-dioxane ring in the chair conformation and the hydroxyl and hydroxymethyl groups in axial and equatorial dispositions, respectively. The Ca^{2+} ions in **2a** and **2b** are bridged by the carbonyl O atoms from two symmetry-related DHA molecules to form centrosymmetric dimers with $Ca \cdots Ca$ distance of 4.307(2) Å in **2a** and 4.330(2) and 4.305(2) Å in two crystallographically independent dimers in **2b**. DHA molecules coordinate to the Ca^{2+} ions by hydroxyl and carbonyl oxygen atoms. The eight-coordinate polyhedra of Ca^{2+} are completed by water molecule and Cl^- ion in **2a** and by four water molecules in **2b**. The dihydroxyacetone molecules in **2a,b**, and **2c** are in an extended conformation, with both hydroxyl groups being *synperiplanar* (*sp*) to the carbonyl O atom. All hydroxyl groups in **2c** (along with water molecules in **2a** and **2b**) are involved as donors in medium strong and weak intermolecular $O-H \cdots O$ hydrogen bonding. Some of them, as well as carbonyl O atoms or Cl^- ions in **2a** and **2b**, act as acceptors in $C-H \cdots O$ (and $C-H \cdots Cl$) hydrogen interactions.

Słowa kluczowe

Sugars, Ketotriose, Dihydroxyacetone, DHA, Dihydroxyacetone dimer, Ca coordination, O–H···O hydrogen bonds, O–H···Cl hydrogen bonds

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