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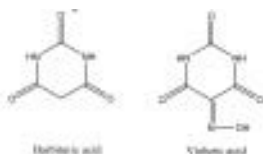
Studies in the Structural Chemistry of Compounds resulting from barbituric and violuric acids

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Barbituric acid is the parent compound for a large variety of derivatives known as barbiturates, widely used for their pharmaceutical properties [1]. Violuric acid is a 5-substituted derivative of barbituric acid. The C=N-OH substituent allows extra coordination and hydrogen bonding possibilities compared to barbituric acid [2].



For some time, an area of our research has concentrated on the synthesis and crystallographic characterisation of s-block metal complexes of these and related ligands. As an extension of this work, we are now studying complexes containing combinations of different ligands.

We present an example of a simple reaction where one equivalent of violuric acid and two equivalents of barbituric acid have been reacted with one equivalent of caesium hydroxide in water, which resulted in three different previously unknown compounds. The structural features observed in each case (coordination, hydrogen bonding etc.) will be discussed as well as the possible mechanisms undergone during the reaction.

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GeO₂ Natrolite-Type Infinite 4 and 8 R-Containing Layers in a 2D Pure-Ge Framework

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Keywords: crystal structure and properties, germanium compounds, layered structures

Our interest is in the influence of the hydroxyl group in the zeotype formation. We have reported the existence of OH anions encapsulated inside the framework cages [1,2], as well as others in which the hydroxyl group is bonded and occupies the fifth coordination position of GeO₄(OH) pentacoordinated species, giving a laminar structure [3], or forms OH-lined 14 R-channels via GeO₂(OH)₂ tetrahedra [4]. Although several zeotypes formed by ethylenediamine have been reported [5-7], none of them has a lamellar structure. Here, we report a new two-dimensional framework germanate ICMM-8, with ethylenediamine-templated 2D structure. Its structural original features are as follows: the arrangement of four and eight tetrahedral ring-containing sheets not previously observed in pure germanium zeotypes and the alternation of [Ge₃O₅(OH)₄]²⁻ infinite inorganic sheets and protonated ethylenediamine cations.

The germanate Ge₃O₅(OH)₄[C₂N₂H₁₀] (denoted ICMM-8), with a 3:9 Ge:O ratio has been synthesized, using a mixture of pyridine, water, and ethanol as the solvent and 1,4-diazabicyclo[2.2.2]octane and ethylenediamine as the structure-directing agents, under solvothermal conditions. The structure was determined by single-crystal X-ray diffraction. In this new compound, the GeO₂ natrolite-type infinite four and eight R-containing layers appears for the first time in a pure GeO₂ framework. The total 2D structure is built up from SBU-6, four tetrahedra, and two octahedra. The hydroxyl groups occupy four positions of each octahedral germanium atom. The compound is characterized by IR spectra and TGA-DTA. Crystal data: Ge₃O₅(OH)₄[C₂N₂H₁₀], monoclinic space group *P*2₁/*c*; *a* = 11.3570(9) Å, *b* = 8.8819(7) Å, *c* = 9.9200(8) Å, β = 90.710(1)°, *V* = 1000.6(1) Å³, *Z* = 4, *R*₁ = 0.044 (*I* > 2(*I*)), and *wR*₂ = 0.1051 (all data).

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