Synthesis and Crystal Structure of SrH$_2$P$_2$O$_6$ · 2 H$_2$O

Introduction

The alkaline-earth metal hypodiphosphates were first reported by Salzer [1]. The crystal structure of hypodiphosphates of alkaline earths are unknown. In our investigations of the chemical behavior of the alkaline earth hypodiphosphates, we have synthesized and structurally characterized the strontium dihydroxy hypodiphosphate dihydrate, SrH$_2$P$_2$O$_6$ · 2 H$_2$O.

The compound crystallizes in the monoclinic space group $C2/c$ with $a = 10.830(4)$, $b = 6.268(1)$, $c = 10.613(3)$ Å, $\beta = 106.95(3)$, $V = 669.3(2)$ Å$^3$ and $Z = 4$.

Experimental

The new hypodiphosphates(IV) hydrate, SrH$_2$P$_2$O$_6$ · 2 H$_2$O, was synthesized by soft chemical reaction from aqueous solution of H$_2$P$_2$O$_6$ · 2 H$_2$O and strontium carbonate at 40 °C. The solution was placed in a vacuum desiccator at 60 °C. After some days standing at this constant temperature colourless plate-shaped crystals of the title compound were obtained from the solution.

The structure was verified by X-ray structure analysis and the Raman spectrum of the title compound was recorded and interpreted.

Structure description

The crystal structure of the title compound is characterized by discrete [H$_2$P$_2$O$_6$]$^{2-}$ anions in staggered conformation, [SrO$_6$] polyhedra and water molecules, held together by hydrogen bonds (Fig. 1 and Tab. 1). The Sr$^{2+}$ cations are eightfold coordinated by O atoms of six anions and two water molecules. The distances between the strontium and the oxygen atoms range between 2.533 and 2.809 Å (Tab. 2), and are thus comparable to those in related compounds, as e.g. SrP$_2$O$_6$ 10 H$_2$O [2]. The coordination polyhedron of Sr$^{2+}$ might be considered as a distorted bicapped trigonal prism (by O1 and O4, CN$_{Sr}$ = 8) (Fig. 2). The water molecules are included in the coordination sphere of Sr$^{2+}$ cation. The main characteristic of the SrH$_2$P$_2$O$_6$ · 2 H$_2$O structure is the [H$_2$P$_2$O$_6$]$^{2-}$ anion. The discrete ethene-like [H$_2$P$_2$O$_6$]$^{2-}$ anions in staggered conformation are on a center of inversion with P – P distances of 2.167 Å. The P – P central bond links two PO$_4$ groups with P – O distances from 1.511 to 1.588 Å. As expected, in SrH$_2$P$_2$O$_6$ · 2 H$_2$O, the bond distances and angles of the [H$_2$P$_2$O$_6$]$^{2-}$ anions are similar of those in Na$_2$H$_2$PO$_4$ · 6 H$_2$O and (NH$_4$)$_2$HPO$_4$ [3, 4].

The hydrogen-bond lengths between O atoms of water molecules and O atoms of [PO$_4$]$^{3-}$ range from 2.644 to 2.802 Å, the O – H – O angles from 161.2 to 176.9 (Tab. 2 and Fig. 3). These values agree very well with those reported previously [5, 6].

The FT-Raman spectrum is presented in Fig. 4. The spectral region below 650 cm$^{-1}$ belongs to [H$_2$P$_2$O$_6$]$^{2-}$, in which the characteristic P – O and P – P stretchings and bendings can be recognized besides the lattice vibrations below about 150 cm$^{-1}$.

References