has a six-pointed starlike shape like ones of hexagonal crystals. We recently examined the structures of the titanium species in the starting solutions and the starlike aggregates. The starting solutions were transparent aqueous ones of crystalline titanate colloids having a layered lepidocrocite-type structure. The starlike aggregates consisted of acicular anatase crystals elongated along the c-axis. The acicular crystals were assembled by oriented attachment and twinning on the {112} planes, to form an arm of the aggregates. The fact that the angle between (112) and (11-2) is about 60° contributes to the six-fold symmetry of the starlike aggregates. In this study, the influence of the type of the tetraalkylammonium hydroxide on the formation of the starlike aggregates was examined in order to elucidate the formation mechanism of the aggregates. TMAOH, $N(C_2H_5)_4OH$ (TEAOH), $N(C_3H_7)_4OH$ (TPAOH) and $N(C_4H_9)_4OH$ (TBAOH) were used as the alkylammonium hydroxide. The use of TMAOH and TEAOH led to the formation of a large number of starlike aggregates. On the other hand, the use of TPAOH and TBAOH decreased the number of the starlike aggregates. It is known that the intercalation of TPA^+ and TBA^+ ions into the interlayer of the lepidocrocite-type titanate leads to exfoliation of the titanate layers. Thus, it is inferred that the layered structure of the colloids in the starting solutions plays an important role in the formation of the six-pointed starlike anatase aggregates.

Keywords: titanium oxide compounds, hydrothermal synthesis, aggregates

P11.10.23

Acta Cryst. (2008). A**64**, C514

A systematic study of the crystal structures of monomethine cyanine dyes

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Cyanines are an important class of dyes which are known for their spectral sensitisation properties and various technical applications. Many of their spectral properties arise from their ability to form aggregates in both solution and on surfaces for which a large number of studies have been made. However there is little information concerning their solid crystalline forms; indeed relatively few examples of their structures are known. For example, in the current version of the CSD there is only one monomethine dye with a simple counterion (Br^-). We have made a systematic study of a series of monomethine crystal structures and present here a survey of their similarities, trends and differences.

Keywords: crystal systematic, dyes, packing analysis

P11.10.24

Acta Cryst. (2008). A**64**, C514

Growth and characterization of new nonlinear optical crystals L-valine and L-valine hydrobromide

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The growth of a new nonlinear optical material L-valine and its inorganic complex L-valine hydrobromide (VHBr) are reported here. The grown crystals were characterized by FTIR, single crystal XRD, DTA-TGA, DSC, optical transmission and second harmonic generation (SHG) efficiency measurement. Bulk single crystals of L-valine and VHBr were grown from their aqueous solution by solvent evaporation method at constant temperature 28°C and 35°C respectively. Single crystal XRD of L-valine and VHBr reveals the lattice parameters to be a = 9.701(3)Å, b = 5.261(2)Å, c = 11.953(2)Å and β = 90.66°(1) for L-valine and a = 10.154(2)Å, b = 7.415(2)Å, c = 5.333(2)Å, and β = 91.22°(2) for VHBr. The result of DTA-TGA study indicates that there is no water of crystallization present in either of the samples. DSC study shows the possibility of phase transition in VHBr.Both the crystals of L-valine and VHBr are optically transparent in the UV-Vis-NIR region with 80% transmission for L-valine and 100% transmission for VHBr. Lower percentage of transmission for crystals of L-valine may be due to poor crystal quality in comparison to VHBr. The second harmonic efficiency of L-valine is 0.82 times that of KDP where as that of VHBr is found comparable to Urea. The above discussion reveals that both L-valine and its derivative VHBr can be used effectively as a new nonlinear optical materials, but the SHG efficiency of VHBr is much higher than that of L-valine. Though L-valine is thermally more stable than VHBr but VHBr is optically more transparent than L-valine as the crystals are superior. The crystals of VHBr are more readily obtained than that of L-valine. Lastly, a probability of phase transition made VHBr a very interesting new NLO material.

Keywords: nonlinear optical materials, crystal growth from solution, characterization

P11.01.25

Acta Cryst. (2008). A**64**, C514

Powder X-ray diffraction of stacking fault containing β -$FeSi_2$

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β-$FeSi_2$ has been studied as thermoelectric materials and optoelectric semiconductor materials. We noticed that the intensities of some specific diffraction peaks were smaller than those calculated with the structure parameters determined by single crystal XRD. We prepared β-$FeSi_2$ from a mixture of Fe and Si at 873-1173 K by using a Na. The powder XRD patterns of the samples were compared with the patterns calculated with DIFFaX for the crystals containing stacking faults. The small diffraction intensities were caused by stacking faults.

Keywords: powder X-ray diffraction, thermoelectric materials, stacking faults in inorganic structures

P11.01.26

Acta Cryst. (2008). A**64**, C514–515

The doubly non-commensurate structure of synthetic tin-selenium cylindrite

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