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Stistaite, an extension of the concept of solid solutions

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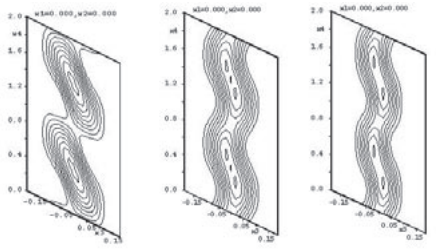
The diffraction patterns from single crystals from Stistaite are dominated by a set of strong reflections that indicate a rhombohedral distortion of a simple cubic lattice. Closer inspection reveals a set of satellites that indicate an incommensurate modulation. The structure of elemental Sb is a simple cubic pattern trigonally distorted by the formation of alternating long and short distances between layers along a cubic <111> direction to yield three long and three short bonds for each Sb atom. The unit cell of elemental Sb is doubled along the trigonal c-axis because of the alternation of interplanar distances. Formally, this may be interpreted as a q-vector of (0 0 1.5) in the rhombohedral unit cell (hexagonal setting). For stistaite, the range of the q-vector is 1.38-1.27 for the composition range 35-55% Sn. The alternating layers of elemental Sb can be interpreted as a saw-tooth like modulation, and for stistaites with a low Sn content, this is largely retained, although the discontinuous portion of the atomic modulation function is smoothened into a sinusoidal region. This corresponds to a part of the structure where Sn and Sb layers alternate with a regular repeat distance.



Modulation functions for Sb (left) stistaite $Sb_{65}Sn_{35}$ (middle) and $Sb_{45}Sn_{55}$ (left)

Keywords: modulated structure, solid solution, stistaite

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Temperature dependence of the modulations in $KNbOB_2O_5$ and $RbNbOB_2O_5$

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$KNbOB_2O_5$ and $RbNbOB_2O_5$ are both members of a family of non-centrosymmetric oxo pyroborates, $AMOB_2O_5$ (A = K, Rb, Cs, Tl; *M* = Nb, Ta) [1-3]. These have attracted considerable interest owing to their potential use as non-linear optical materials. If one considers the structure of $CsNbOB_2O_5$ [4] as the underlying average structure, it is then possible to describe the structures of all other members of that family as modulated variants thereof. The structures of, *e.g*., $KNbOB_2O_5$ [1] and $RbNbOB_2O_5$ [2] have been refined using a super space approach. The structure of $RbNbOB_2O_5$ is incommensurately modulated, despite the apparent value of the modulation wave vector of 2/5 **b*** exactly, while the structure of $KNbOB_2O_5$ refined significantly better as commensurate modulated structure. Using metrics alone it is not straightforward to determine whether a structure is commensurately or incommensurately modulated, however, a variability of the magnitude of the modulation wave vector with composition (*e.g*. for solid solutions) or temperature may be used to resolve the ambiguity. Variable temperature X-ray powder diffraction data were collected for both $KNbOB_2O_5$ and $RbNbOB_2O_5$ at the Australian National Beamline Facility, Photon Factory, Tsukuba, Japan. Diffraction patterns were collected at RT and from 423 K to 1073 K in 25 K steps. The results of the analysis of these data, which supports the previously suggested reason for the modulation, will be presented here.

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Keywords: modulated structure, powder diffraction, temperature dependence

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X-ray structural analysis and biophysical assays in drug discovery

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Examples of the combined use of biophysical assays and X-ray structures of target complexes for drug discovery will be presented.

Keywords: Biacore, drug discovery, ITC

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Studies of protein-protein and protein-RNA complexes by mass spectrometry

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Electrospray ionization mass spectrometry (ESI-MS) enables the determination of not only the molecular sizes of non-covalent macromolecular complexes, but also the binding affinities. This paper shows the advantages of ESI-MS over other techniques in structural studies of biological macromolecular complexes, using as an example our recent analysis of TRAP, trp RNA-binding attenuation protein, and its complexes with RNA and protein ligands. TRAP and its regulator anti-TRAP protein (AT) play the principal roles in controlling tryptophan synthesis in *Bacillus* species. We have characterized both wild-type (wt) and mutant TRAP from *B. stearothermophilus*, and their complexes with RNA or AT by ESI-MS. Wild-type TRAP forms homo-11mer rings. The mutant used carries three copies of the TRAP monomer on a single polypeptide chain, so that it associates to form a 12mer ring with four polypeptides. Mass spectra showed that both the wt TRAP 11mer and the mutant TRAP 12mer can bind a cognate single-stranded RNA. The crystal structure of wt TRAP complexed with AT shows a TRAP 12mer ring surrounded by six AT trimers. However, ESI-MS of wild-type TRAP mixed with AT shows four species with different binding stoichiometries, and the complex observed by crystallography