Supplementary material

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$Na_2Si_3O_7$: An incommensurate structure with crenel-type modulation functions, refined from a twinned crystal

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Abstract

The structure of metastable, incommensurately modulated $Na_2Si_3O_7$ has been determined from single crystal X-ray diffraction data. In contrast to previous investigations which stated that the compound crystallises orthorhombic, this study shows that the compound is monoclinic with a pseudo orthorhombic cell and is affected by twinning. The structure is described in the (3+1)-dimensional superspace. Crenel-type modulation functions are used to account for an aperiodic sequence of enantiomorph oriented *zweier* single chains of silicate tetrahedra. The modulation mainly affects one of the two symmetrically independent tetrahedral chains, which are connected to build up $[Si_3O_7]^{2-}$ layers. Sodium cations are coordinated by five oxygen ligands and provide linkage between adjacent tetrahedral sheets. Distortions of the silicate tetrahedra and crystal chemical relationships of the title compound to sodium and lithium di- and metasilicates are discussed in detail.

Figure 1: Bond valence sum of Si1. The constant line represents the unmodulated value, the averaged value is lower at 4.07(10).

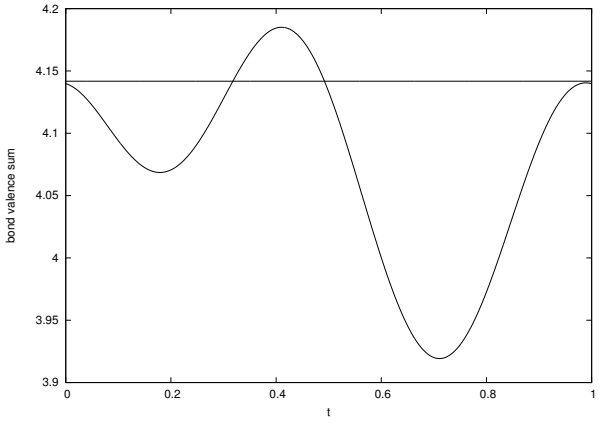

Figure 2: Modulated O-Si1-O bonding angles. Constant lines represent unmodulated angles.

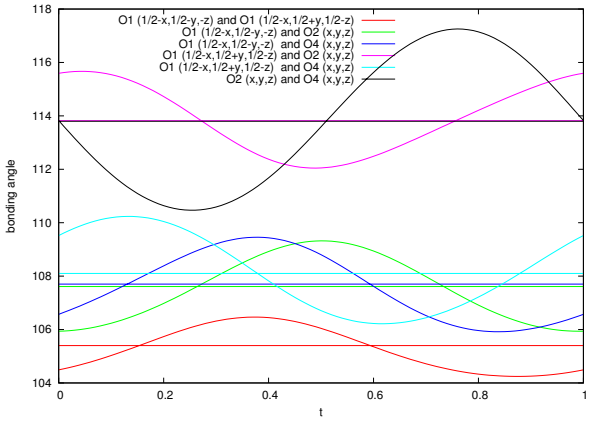

Figure 3: Modulated O-O bonding angles in Si1 tetrahedra.

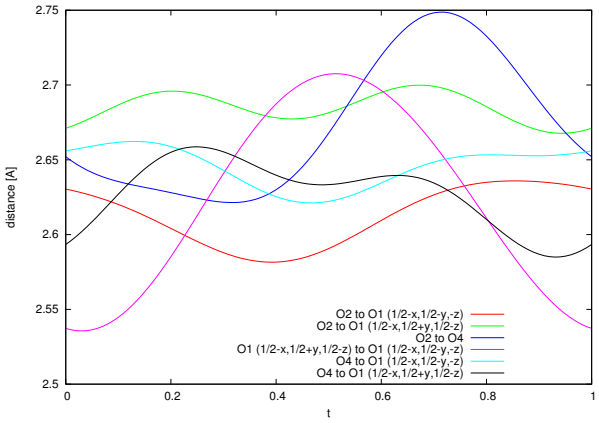

Figure 4: Modulated volume of Si1 tetrahedra.

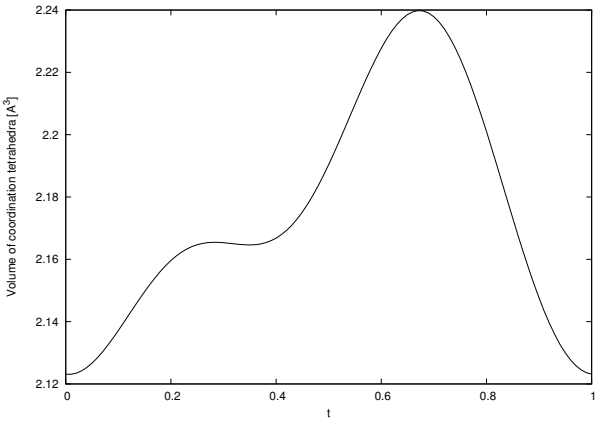

Figure 5: Quadratic elongation of Si1 tetrahedra.

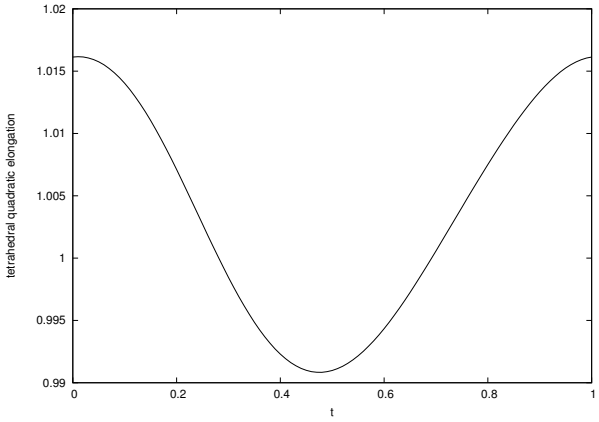

Figure 6: Tetrahedral angle variance of Si1 tetrahedra.

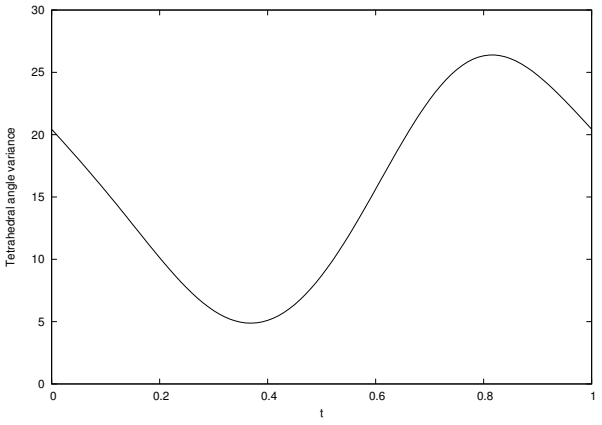

Figure 7: Bond valence sum of Si2. The constant line represents the unmodulated value, the averaged value is lower at 4.28(10).

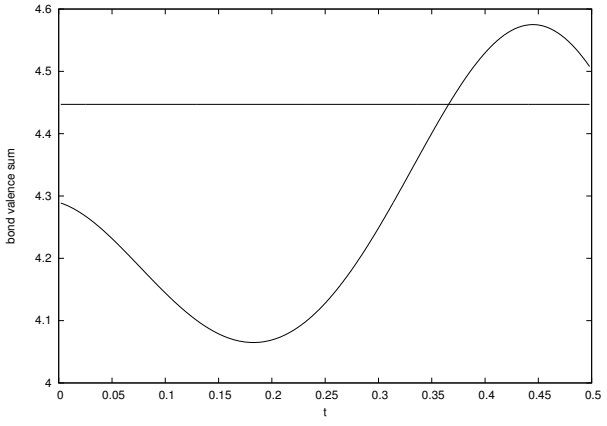

Figure 8: Modulated O-Si2-O bonding angles. Constant lines represent unmodulated angles.

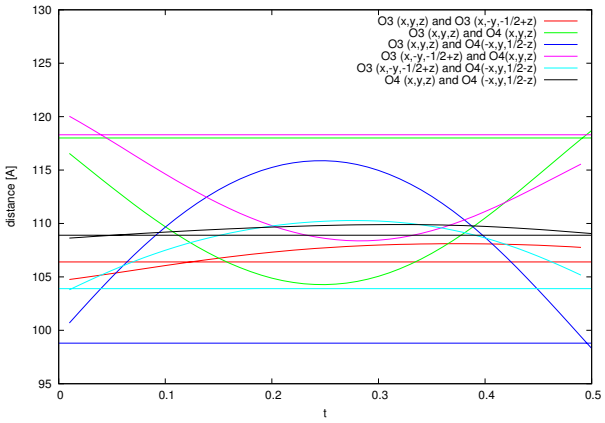

Figure 9: Modulated O-O bonding angles in Si2 tetrahedra.

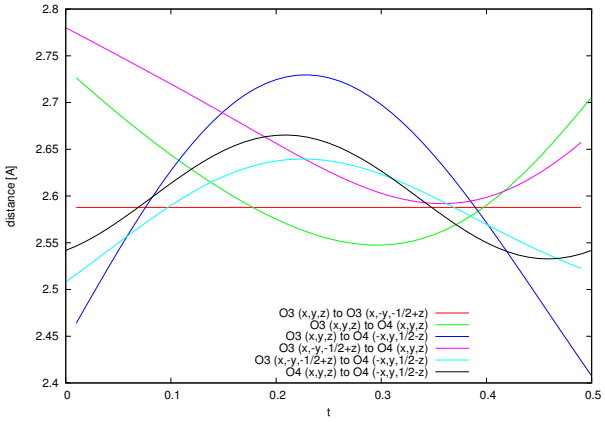

Figure 10: Modulated volume of Si2 tetrahedra.

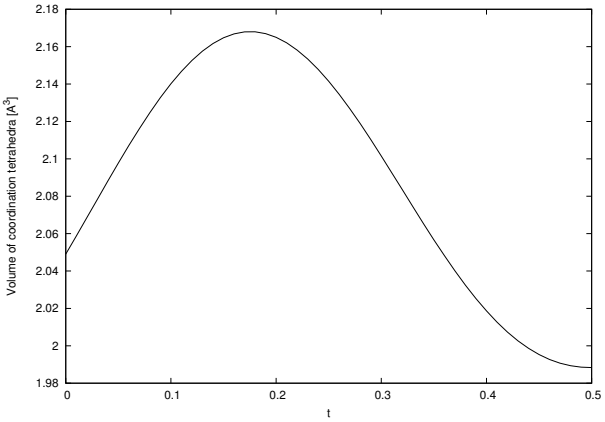

Figure 11: Quadratic elongation of Si2 tetrahedra.

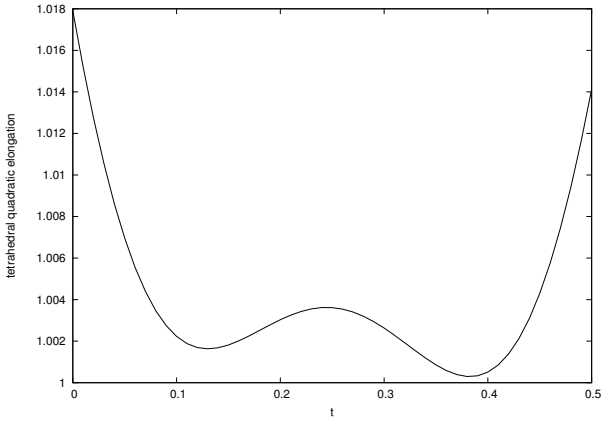

Figure 12: Tetrahedral angle variance of Si2 tetrahedra.

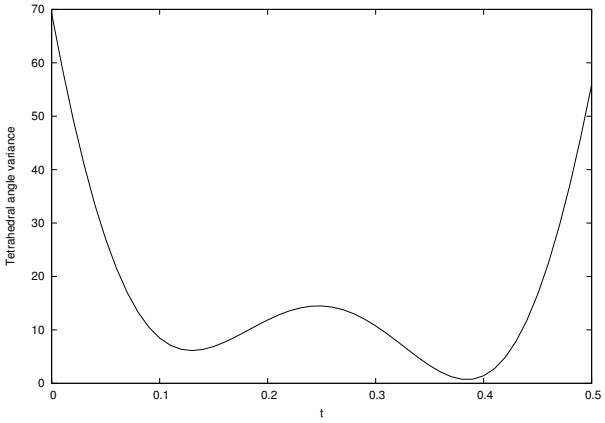

Figure 13: Bond valence sum of the sodium atom Na1. The constant line represents the unmodulated value, the averaged value is at 1.01(8).

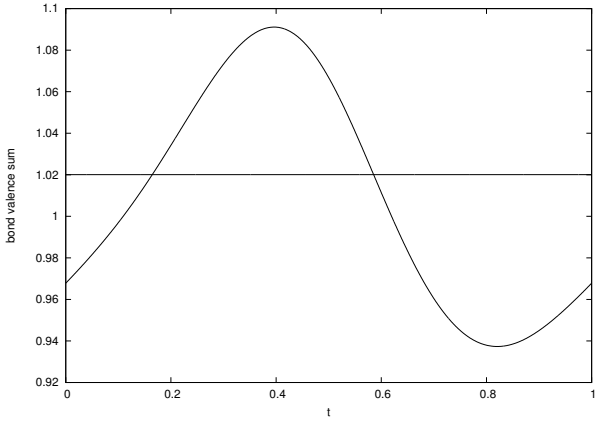

Figure 14: Modulated Na1-O distances. Constant lines represent unmodulated distances.