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AB-INITIO DETERMINATION OF $Na_2Si_3O_7$ FROM CONVENTIONAL POWDER DIFFRACTION DATA

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The crystal structure of $Na_2Si_3O_7$ has been determined by direct methods using integrated intensities of conventional powder diffraction data and subsequently refined with the Rietveld technique. The title compound was prepared from $Na_2Si_3O_7*H_2O$ by careful thermal decomposition at 440°C. Sodium trisilicate adopts monoclinic symmetry, space group $P2_1/c$ with unit cell parameters a = 7.1924(5)Å, b = 10.6039(8)Å, c = 9.8049(7)Å, β = 120.2478(4)°, V = 646.0(9)Å^3 and Z = 4. It belongs to the group interrupted framework silicates of four- and three-connected [SiO_4]-tetrahedra with a ratio of Q^3:Q^4 = 2:1. There exist different possibilities to subdivide the interrupted framework structure of $Na_2Si_3O_7$ into tetrahedral layers which build up the whole network by corner sharing.

Figure 1 shows the connectivity between the Si-atoms of a single tetrahedral layer perpendicular to [001] in sodium trisilicate. Within the corrugated sheet, chains can be isolated which consist of four-membered (S4R) and six-membered (S6R) rings. At the interface between neighboring chains, S8R are formed. Each S4R consists of two Q3 and two Q4 groups, whereas a single S6R contains four Q^3 and two Q^4. A projection of $Na_2Si_3O_7$ parallel to [100] is given in Figure 2. As can be seen the framework contains channels running along *a* with pore openings formed by ten-membered rings. Charge balance within the structure is achieved by the incorporation of sodium atoms which are coordinated by 4 to 6 oxygen ligands. The Na2 atoms are located within the central regions of the tunnels mentioned above, whereas the Na1 ions occupy positions closer to the boundary of the channels. The porous character of the new phase is reflected in a framework density FD = 18.6 T-atoms/1000 Å^3, a value which is comparable to those observed in zeolitic materials.

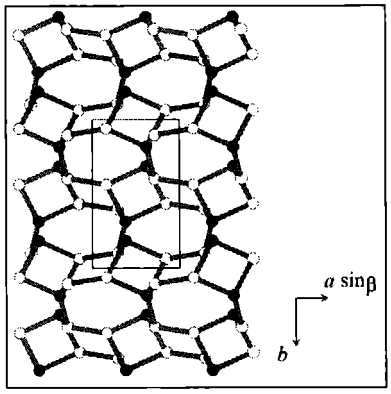

Fig. 1
Projection of a single tetrahedral layer parallel to [001]. Q^4- and Q^3-atoms are represented by black and white spheres, respectively.

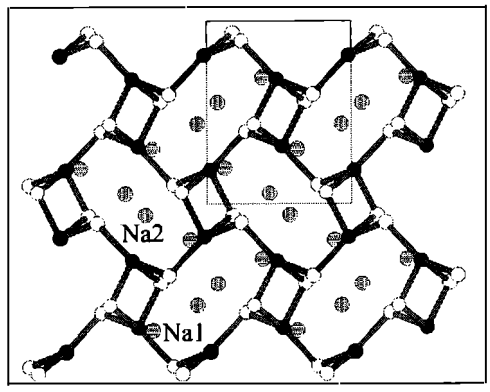

Fig. 2
Projection of the framework parallel to [100].