Ab initio crystal structure determination of Na2Si3O7 from conventional powder diffraction data

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The crystal structure of Na2Si3O7 has been determined by direct methods using integrated intensities of conventional X-ray powder diffraction data and subsequently refined with the Rietveld technique. The title compound was prepared from Na2Si3O7 × H2O by careful thermal decomposition at 440°C. Sodium trisilicate adopts monoclinic symmetry, space group P21/c with unit cell parameters a = 7.1924(5) Å, b = 10.6039(8) Å, c = 9.8049(7) Å, ? = 120.2478(4),° V = 646.0(9) Å3 and Z = 4. It belongs to the group of interrupted framework silicates of four- and three-connected [SiO4]-tetrahedra with a ratio of Q3:Q4 = 2:1. Within the framework the sodium atoms are coordinated by 4 to 6 oxygen ligands. The porous character of the new phase is reflected in a framework density FD = 18.6 T-atoms/1000 Å3, a value which is comparable to those observed in zeolitic materials. The topology of the tetrahedral network is identical to the one observed in the hydrous sodium silicate Na2Si3O7 × H2O. Differences