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$Cs_3ScSi_8O_{19}$, A NEW MICROPOROUS SILICATE WITH EIGHT-MEMBERED RINGS

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During investigations of the system Sc_2O_3-Al_2O_3-TiO_2-SiO_2, which contains several important ceramic phases, a new microporous compound, $Cs_3ScSi_8O_{19}$, was synthesized as colourless, glassy plates from a CsF-MoO_3 flux. The crystal structure was determined from single-crystal X-ray diffraction data (Mo-Kα radiation, CCD area detector, $2\theta_{max} = 60°$, $R_{int} = 1.3$ %). The compound is orthorhombic, space group *Pnma*, with a = 11.286(2), b = 7.033(1), c = 26.714(5) Å, and Z = 4 (R1 = 2.6 % and $wR2_{all} = 7.3$ % for 3066 'observed' reflections with $F_o > 4\sigma(F_o)$).

The structure of $Cs_3ScSi_8O_{19}$ represents a novel, mixed octahedral-tetrahedral framework structure type. It is based on isolated, nearly regular ScO_6 octahedra [d_{av}(Sc–O) = 2.112 Å] sharing corners with SiO_4 tetrahedra to form an open framework with four-, six- and eight-membered rings; the latter are composed of SiO_4 tetrahedra only. Three non-equivalent Cs atoms occupy large voids in the framework, close to the puckered eight-membered rings. The voids are connected into channels running along several directions. One Cs position is split into four partially occupied and disordered sites. Determinations of the unit-cell parameters at 120 K suggest no phase transition, and an only very small volume shrinkage of ca. 0.4 %.
The structure is compared with that of the structurally related compound $Cs_2TiSi_6O_{15}$ [1, 2] and with other natural and synthetic microporous titano- and zircono-silicates, which recently have attracted considerable interest due to their microporous properties, e.g. [3]. $Cs_3ScSi_8O_{19}$ or derivatives may be important in the context of immobilisation of radioactive Cs waste, cationic conductivity or catalysis.

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References

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