HYPOTHETICAL FRAMEWORK STRUCTURES RELATED TO MOBIL ZEOLITE ZSM-48. By J.L. Schlenker and W.J. Rohrbach, Mobil Research and Development Corporation, Research Department, Paulsboro, NJ 08066, USA. ZSM-48 is a high-silica zeolite whose structure has been proposed to be a disordered linking of ferrierite sheets via bridging oxygen atoms located on mirror planes. The proposed framework topology was based on agreement observed and calculated x-ray powder diffraction patterns. The Smith plot in best agreement was obtained from a disordered intergrowth of two ideal framework structures with Caca and Imma symmetries. Because x-ray and electron diffraction data seem to indicate an orthorhombic lattice with pseudo-I or pseudo-C-centering, attention was initially restricted to the formulation of hypothetical centered structures. With lattice parameters of a=14.24 A and b=20.14 A, and a C-center, the orthorhombic lattice has only four independent T-atoms, each of which may point up (U) or down (D) in order to link with other sheets. Alternating the orientation of these independent T-atoms yields twenty-eight closely related hypothetical framework structures, e.g. UDDD-Caca, UUUD-Imma, etc.


Octahedrally shaped crystals of the zeolite up to 0.7mm in size were grown hydrothermally from a gel with a composition 3Na2O.16TMA0.0: 16(TMA)2:0.1 A12O3.11OSIO4.0:22H20/SiO2, for 7 days at 473 K. A spherically ground transparent crystal with r = 0.19mm was investigated on a CACABED diffractometric system. Crystal data: (Na,TMA)4.4A14.5131.0 272, Mr = 6337, cubic, Fd3m, a = 19.396(1) A, V = 7297(1) A3, Z = 1, D, = 1.897 g.cm-3, (MoKα) = 0.71073 A, μ = 6.8 cm-1, F(000) = 4180, T = 291 K. From 8958 total (d=0.5) and 316 unique (R=0.053) reflections with l>2σ(l) were used in calculations. Final R(F) = 0.035 by full-matrix least-squares. Residual max. Δ(p)= 0.09 e.A-3.

The ZSM-39 topology, known from the powder data study (Schlenker et al., Nature, 1981, v. 294, 540-2) was confirmed. Besides, disordered Al, Na and TMA were localized in the 16-hedral cage. The Al-atom occupies a tetrahedron which shares face with another, currently vacant SiO4-tetrahedron from the framework. The apical oxygen atom of AlO4 is pointed to the centre of the cage, where both the Na and TMA are disposed. The electron density peak near the centre of the 12-hedral cage is presumably a water-oxygen.