PA2 THE CRYSTAL STRUCTURE OF MONOCLINIC ANCYLITE,

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The structure of ancylite from Mont St. Hilaire, Québec, was first described[1] on the basis of an orthorhombic cell, *Pmcn*, despite the fact that an earlier report[2] had given the space group as *Pmmm* (no absences). One of us (GYC) examined over 50 crystals from the same locality, and found no systematic absences in the data, consistent with the earlier space group. However, apparent streak-lengthening in precession-orientation photographs, and optical anomalies, suggested that these crystals were twinned monoclinic. Successive division of a crystal produced one fragment with monoclinic symmetry and no systematic absences: a=7.264(2), b=5.021(1), c=8.512(2)Å, β=90.32(1)°. This cell can be derived by an angular distortion from the *Pmcn* cell, when the latter is transformed to the more conventional *Pnma* setting. The unique quadrant of data was obtained by averageing the whole MoKα sphere to 2θ=80°, (2072 refl, 7 unobs., space group *Pm*). Analysis of fragments from the same crystal show the metal composition as $(Ce_{1.48}La_{0.72}Pr_{0.20}Nd_{0.16}Gd_{0.08})$ ΣRE=2.64, $(Sr_{0.68}Ca_{0.66}Ba_{0.02})$ ΣAE=1.36, RE=Rare Earth, AE=Alkali Earth. From the fourfold equipoint of *Pnma*, the metal sites are now independent, and LS refinement of the AE and RE population parameters reveals major ordering of AE/RE between the four sites, so that AE preferentially occupies one site (AE/RE=0.919/0.081), the other sites having 0.095/0.905, 0.125/0.875, 0.218/0.782. The chemical formula, derived from the structure analysis, is $(AE,RE)(RE,AE)_3(CO_3)_4(OH,F,H_2O)_4$. Refinement converved to R=3.17%. The monoclinic *Pm* structure is derived from a distortion of the *Pnma* model, with significant differences in the metal-oxygen 10-fold coordination polyhedra.

1. Dal Negro, A., Rossi, G. & Tazzoli, V. (1975): *Amer. Mineral.* 60, 280-284.
2. Mandarino, J.A., Harris, D.C. & Bradley, J. (1965): *Can. Mineral.* 8, 398.

PA3 $Li_4Ge_5O_{12}$, A NEW OPTICALLY INTERESTING Li-Ge-O PHASE

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Crystals of a previously unreported phase of lithium germanate, $Li_4Ge_5O_{12}$ have been grown and the crystal structure determined. The crystals are triclinic, space group P1 with Z=2 and Dx=4.66 gr/cm^3. The structure can be described as consisting of quasi-close-packed planes of oxygens bonded to one another by Ge and Li cations. Four Ge/unit-cell are tetrahedrally coordinated with <Ge-O>=1.75Å and six Ge/unit-cell are octahedrally coordinated with <Ge-O>=1.90Å. Faint superlattice reflections on long-exposure rotation photographs indicate some additional ordering.

Crystals up to 1.5 cm in diameter and 4.0 cm in length were pulled at 1 mm/hr from a melt of composition $Li_6Ge_8O_{19}$ at 953°C. The existence of $Li_4Ge_5O_{12}$ as an equilibrium phase requires the modification of the GeO_2 rich end of the Li_2O-GeO_2 phase diagram. When the melt is doped with 0.01 - 0.3% Ti^{+4} the resulting crystals exhibit broad band luminescence from about 388 - 524 nm.

For the structure determination 2918 reflections were measured using MoKα radiation in the 2θ range 3°-50°. An empirical absorption correction was applied to the data which was obtained from a spherical crystal 0.35 mm in diameter. The 10 Ge positions were generated from a Fourier synthesis of selected, phased structure factors obtained using the program RANT from the SHELXTL software package. Difference Fouriers then yielded the 24 O positions and 8 Li positions. Final $R = [\Sigma|Fo - Fc|/\Sigma|Fo|] = 2.77\%$ Lattice constants of $Li_4Ge_5O_{12}$ are a=5.120(2)Å, b=9.143(3)Å, c=9.586(3)Å, α=72.95(1)°, β=77.74(1)° and γ=78.81(1)°.

PA4 POWDER NEUTRON DIFFRACTION STUDIES OF LITHIUM AND SILVER EXCHANGED ZEOLITE RHO.

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The structures of dehydrated lithium and silver exchanged zeolite rho have been studied by powder neutron diffraction. The atom positions and profile parameters were refined using the curve fitting procedure originally devised by Rietveld. The aluminosilicate framework is quite different from that found in other variants of zeolite rho and illustrates the flexibility of this particular structure. The double-8-rings are elliptical with their major axes perpendicular. This results in an almost ideal tetrahedral site at the midpoint of the two rings. The framework distortions reduce the symmetry of the system giving rise to the non-centrosymmetric space group $I\bar{4}3m$ and the anomalously small unit cell dimensions. The cell length, a, is 14.493(1)Å for lithium and 14.225(1)Å for silver rho. The latter is the shortest yet reported. Lithium is located at the center of the single-6-ring, while silver prefers the four-fold coordination associated with the single-8-ring.

Our aim when starting these studies was to investigate how the cation site preference in zeolite rho alters pore dimensions and void characteristics. The ability to manipulate channel openings and so restrict access to the active centers has long been recognized as a major step to achieving more selective and efficient catalysts. The rho structure seems particularly amenable to studies of this kind because of the ease with which one can distort the aluminosilicate framework.

PA5 STRUCTURE AND COMPOSITION OF JUVINAS CHONDRITIC PLAGIOCLASE.

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Plagioclase feldspar minerals of Juvinas chondritic meteorite shows wide range of anorthite content indication the impact mixing of the various chemical sources.

Juvinas plagioclase $(Ca, Na, K, Fe, Mg)(Si, Al, Fe, Mg)_4O_8$ indicates the substitution of Fe and Mg ions in Si-tetrahedral and Ca sites. The minor contents of Fe and Mg substitutions affect the cell-volume and atomic distances. The mean distance of T-O distance is decreased up to 1.663 Å (compared with the terrestrial anorthite, 1.681 Å), whereas that of Ca-O distance is increased up to 2.538 Å (cf. 2.493 Å of the terrestrial one). The shortest and longest atomic distances are obtained in T2(OO)-OA(20) and Ca(zi)-OD(mz), respectively.

The complicated behavior of atomic distances in the Juvinas plagioclase is due to the atomic substitution. Crystal data: $(Ca, Na, K, Fe, Mg)(Si, Al, Fe, Mg)_4O_8$, triclinic, $P\bar{1}$, a = 8.182(4), b = 12.844(12), c = 14.146(7), α = 93.23(2), β = 115.96(4), γ = 91.12(3), V = 1329.5Å^3, Z = 4, R = 0.152 for 8680 observed reflections collected with a Rigaku AFC-5FDOC four-axes diffractometer at room temperature using MoKα monochrometer.