REFINEMENT OF THE CRYSTAL STRUCTURES OF COEXISTING MUSCOVITE AND PARAGONITE

by

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EXTENDED ABSTRACT

THE CRYSTAL structures of specimens of muscovite and paragonite coexisting in a mica–kyanite schist from Alpe Sponda, Switzerland, have been refined using three-dimensional least-squares techniques. Anisotropic thermal models yield identical R values of 0.038 for 619 muscovite observations and 558 paragonite observations. Refinement of the occupancies of K and Na in the interlayer cation positions gives compositions corresponding to $Mu_{66}Pa_{34}$ for muscovite and $Mu_{13}Pa_{87}$ for paragonite; these results agree with compositions calculated from electron-microprobe analyses of these materials.

Direct comparison of atomic co-ordinates shows that the two crystallographically independent tetrahedral cations are coplanar in both structures, as are the two independent tetrahedral apical oxygen atoms. Within the surface oxygen layer, two of the three independent oxygen atoms are coplanar in both structures. The differing z-co-ordinates of the third oxygens correspond to departures from coplanarity normal to the sheet of 0.266Å (muscovite) and 0.238Å (paragonite). Thus the basal oxygen layer is rippled, or corrugated, by the tilting of each tetrahedron. The extent of corrugation is slightly, but probably significantly, greater in paragonite than muscovite.

Average T—O (T = tetrahedral cation) interatomic distances are 1.645Å and 1.645Å in muscovite, 1.652Å and 1.651Å in paragonite. These averages demonstrate conclusively that, in both structures, each tetrahedron contains a disordered arrangement of Si and Al atoms corresponding to the composition (Si_3Al). The difference of 0.006Å between the muscovite and paragonite averages, results from slight rearrangement of the surface oxygen layers as Na substitutes for K in the interlayer cation position. In muscovite the average of six alkali—O distances is 2.793Å; this decreases to 2.641Å in paragonite.

Structural differences between the two minerals are primarily restricted to the surface oxygen layers. The dioctahedral layers have average Al–O distances of 1.923Å in muscovite and 1.913Å in paragonite; and average O—O distances of 2.824Å (muscovite) and 2.807Å (paragonite) for nine unshared edges, and 2.420Å (muscovite) and 2.417Å (paragonite) for three shared edges.

Thermal models for both structures are very similar. Substitutional disorder in the tetrahedral and interlayer cation positions causes abnormally large rms displacements of co-ordinating oxygen atoms toward these cations.

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https://doi.org/10.1346/CCMN.1964.0130103 Published online by Cambridge University Press

Lattice constants and individual interatomic distances have been given previously (Burnham and Radoslovich, 1964). A detailed report of this study is now in preparation.

REFERENCE

BURNHAM, C. W., and RADOSLOVICH, E. W. (1964) The crystal structures of coexisting muscovite and paragonite, Carnegie Inst. Washington Year Book 63, pp. 232–6.

https://doi.org/10.1346/CCMN.1964.0130103 Published online by Cambridge University Press