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Fe-Mg order-disorder in tremolite–actinolite–ferro-actinolite at ambient and high temperature

Bernard W. Evans[1] and Hexiong Yang[2]

[1] Department of Geological Sciences, Box 351310, University of Washington, Seattle, Washington 98195-1310, U.S.A.
[2] Geophysical Laboratory, 5251 Broad Branch Road, NW, Washington, D.C. 20015-1305, U.S.A.

Abstract

The crystal structures and M-site populations of a series of unheated and heat-treated, near-binary members of the actinolite series were determined from single-crystal X-ray diffraction data. Small, systematic differences in crystal structure (mean and individual bond lengths, octahedral distortions, and Mg-Fe site preferences) between the actinolite and cummingtonite series are documented and rationalized in terms of the bond-valence model. Mg-Fe^{2+} site preferences among the M1, M2, and M3 sites in the actinolite series are small. Between M1 and M3, site preference (Fe^{2+} slightly in favor of M1) is independent of temperature. Mg is favored in M2 over M1 in unheated samples (less strongly than in cummingtonite-grunerite), but Fe^{2+} and Mg are virtually disordered in samples re-equilibrated at 700 °C. Site preference between M2 and M3 and possibly also between M1 and M2 appears to undergo a reversal as a result of heat treatment, but consideration of all sources of error renders this conclusion a tentative one, although the observation could be explained in terms of a bond valence deficiency. The ratio of Fe^{2+}/Mg atoms on M4 cannot be accurately determined, but refinements indicate that, like cummingtonite-grunerite, it is larger than on all other M sites. Expansion of the cell dimensions with an increase in Fe/Mg ratio follows a pattern similar to that of thermal expansion, and a and β are influenced by cummingtonite-grunerite solid solution. The data are consistent with a cell volume of 942.8 $Å^3$ (or molar volume of 2.8388 J/bar) for end-member ferro-actinolite, a first approximation that assumes a reciprocal, quadrilateral ΔV of zero.