Octahedral site Fe^{2+} quadrupole splitting distributions from the Mössbauer spectra of arrojadite

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ABSTRACT

The Mössbauer spectra of arrojadite, $(K,Ba)(Na,Ca)_5(Fe^{2+},Mn,Mg)_{14}Al(PO_4)_{12}(OH,F)$, at 298 and 95 K were investigated for the first time. The spectra at both temperatures were analyzed in terms of their Fe^{2+} quadrupole splitting distributions (QSDs). The overall QSDs at both temperatures can be interpreted in terms of five octahedral site Fe^{2+} QSD contributions. The quadratic elongation, $\langle\lambda\rangle$, and the variation of bond angles, σ^2, for the different sites were calculated on the basis of the structural data obtained by Moore et al. (1981). The five QSD contributions are tentatively assigned to Fe^{2+} in the M3, M4, M5, M6, and M7 sites, based on the structural determination and the relation of the quadrupole splitting to the distortion of the octahedra, respectively. The Fe^{2+} ions are randomly distributed over the M3, M4, M5, M6, and M7 sites. In addition, Mössbauer data from arrojadite and related phosphate minerals indicate that the mean value of the isomer shift of Fe^{2+} in the octahedral sites in phosphate minerals is ~ 0.07 mm/s larger than that in silicate minerals. This difference is explained in terms of electron affinity.