American Mineralogist, Volume 85, pages 943–952, 2000

Temperature dependence of the hyperfine parameters of synthetic $P2_1/c$ Mg-Fe clinopyroxenes along the $MgSiO_3$-$FeSiO_3$ join

S.G. EECKHOUT,[1,*] E. DE GRAVE,[1,†] C.A. MCCAMMON,[2] AND R. VOCHTEN[3]

[1]Department of Subatomic and Radiation Physics, University of Gent, Belgium
[2]Bayerisches Geoinstitut, University of Bayreuth, Germany
[3]Department of Chemistry, University of Antwerp, Belgium

ABSTRACT

Transmission ^{57}Fe Mössbauer measurements were acquired in the temperature range 11–745 K from a suite of nine synthetic Ca-free $P2_1/c$ Mg-Fe clinopyroxenes (cpx) along the $MgSiO_3$-$FeSiO_3$ join. The paramagnetic Mössbauer spectra (MS) consist of one doublet produced by Fe^{2+} ions at an almost regular octahedral M1 site and a second doublet at a more distorted octahedral M2 site. The temperature dependencies of the Fe^{2+} center shifts were fit to equations derived from the Debye model for the lattice vibrations, allowing the determination of the characteristic Mössbauer temperatures for the two Fe sites. The temperature variations of the M1 and M2 quadrupole splitting $\Delta E_Q(T)$ are consistent with the higher distortions of the M2 octahedra. Applied-field MS revealed that the principal component of the electric field gradient, V_{zz}, is positive, implying a tetragonal compression of both octahedral sites. The crystal-field model was used to analyze $\Delta E_Q(T)$ and to calculate the energy gaps Δ_1 and Δ_2 of the first excited electronic states within the ^{5}D orbital term, both at M1 and M2. The various physical quantities derived from the MS are discussed in terms of the Fe/(Fe + Mg) ratio.