

Mössbauer spectroscopy of Zn-poor and Zn-rich rhodonite

DANA T. GRIFFEN* AND WENDY R. NELSON†

Department of Geological Sciences, Brigham Young University, Provo, Utah 84602, U.S.A.

ABSTRACT

Room-temperature Mössbauer spectra of five specimens of typical, Zn-poor rhodonite and five of Zn-rich rhodonite (“fowlerite”) have been obtained to determine whether the spectra reflect structural differences between the two varieties. All Fe is divalent and in the high spin state, and the spectra support the interpretation that Fe is present in all five M sites. Assignment of Mössbauer doublets to specific sites is made principally on the basis of isomer shift values and relationships between quadrupole splitting and polyhedral distortion parameters determined from previously reported crystal-structure refinements. Trends in Mössbauer parameters show correlations with trends in steric details of the sites, both among individual M sites within Zn-rich and Zn-poor varieties and between corresponding M sites of rhodonite and fowlerite. In particular, the Mössbauer parameters for the geometrically similar M1 and M2 sites are similar, and those of M4 and M5 reflect the tendency of the former toward more tetrahedral character and the latter toward less distortion in fowlerite. Iron occupancy is largely a function of polyhedral volume, although there is a secondary preference for octahedral coordination. Structural differences previously determined between rhodonite and fowlerite, which are driven principally by high concentrations of Zn in M4 and Ca in M5, are structurally pervasive and are maintained even when Fe substitutes for Zn or Ca.

Keywords: Rhodonite, fowlerite, Mössbauer spectroscopy, pyroxenoid