Part III: Crystal Structure of Pyroxferroite

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A crystal structure analysis of pyroxferroite is proceeding on the basis of some 10,000 independent hkl intensity measurements carried out on a single-crystal obtained from rock 10047. Unit cell dimensions and diffraction patterns of pyroxferroite are very similar to those of synthetic Ca$_{15}$Fe$_{.85}$Si$_{10}$O$_{3}$ (Lindsley and Burnham, 1970). The diffraction intensities display a definitely centrosymmetric triclinic distribution; the space group is $\overline{P1}$, and $Z$ for a formula based on three oxygens is 14. A solution of the structure is being carried out without reference to the ill-defined Liebau (1959) structure of presumably isostructural pyroxmangite. Symbolic addition methods have yielded most of the expected features of the octahedrally coordinated metal layer. Fourier techniques are being used to determine additional oxygen positions and the silicate chain configuration. Since there are seven crystallographically independent sites for metals other than Si, the compositional ratio Ca/(Ca+Fe) suggests that Ca is constrained to one of these, with Fe$^{2+}$ and minor Mg and Mn$^{2+}$ occupying the other six sites. The bond distances required to confirm this scheme will be available soon.