American Mineralogist, Volume 85, pages 473–479, 2000

Raman spectroscopic characteristics of Mg-Fe-Ca pyroxenes

E. HUANG,* C.H. CHEN, T. HUANG, E.H. LIN, AND JI-AN XU

Institute of Earth sciences, Academia Sinica, Taipei 115, Taiwan

ABSTRACT

Raman spectra of several compositions of (Mg, Fe, Ca)SiO_3 pyroxenes were collected at ambient conditions. More than 10 Raman vibrational modes were observed for these pyroxenes in the wavenumber range between 200 and 1200 cm^{-1}. In general, these pyroxenes are characterized by (1) the Si-O stretching modes above 800 cm^{-1}; (2) the Si-O bending modes between 500 and 760 cm^{-1}; (3) SiO_4 rotation and metal-oxygen translation modes below 500 cm^{-1}. For a constant Ca content, frequencies of the Raman modes in the enstatite-ferrosilite (opx) and diopside-hedenbergite (cpx) series generally decrease with an increase in Fe content. This phenomenon is attributed to an increase in both the bonding lengths and the reduced mass as Fe^{2+} is substituted for Mg. However, two modes at ~900 cm^{-1} in the enstatite-ferrosilite series increase in frequencies as Fe content increases. A possible explanation is to the shortening in the Si-O-Si bridging bonding bonds when the M2 sites are preferentially occupied by the iron cation. The effect of Fe substituting for Mg on the frequency shift in cpx is less profound than opx because the larger M2 was occupied by calcium and the substitution of iron and magnesium in the M1 site results in a less significant change in the bond length. The major-element composition of the (Mg, Fe, Ca)-pyroxenes, especially the orthopyroxene series, can be semi-quantitatively determined on the basis of the peak positions of their characteristic Raman modes.