American Mineralogist, Volume 92, pages 1492–1501, 2007

The crystal structure of pyroxenes along the jadeite–hedenbergite and jadeite–aegirine joins

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Abstract

The crystal-structures of seven synthetic pyroxenes along the jadeite–hedenbergite ($Jd_{57}Hd_{43}$, $Jd_{26}Hd_{74}$, $Jd_{0}Hd_{100}$) and jadeite–aegirine ($Jd_{100}Ae_{0}$, $Jd_{76}Ae_{24}$, $Jd_{35}Ae_{65}$, $Jd_{0}Ae_{100}$) joins were refined using data collected by means of single-crystal X-ray diffraction (space group $C2/c$, $R_{4\sigma}$ between 2.2 and 3.4%).

The M2 and M1 polyhedral volumes and bond lengths increase with increasing aegirine and hedenbergite content, moreover the Ca for Na substitution along the jadeite–hedenbergite join changes the M2 coordination from 6 + 2 to 4 + 4, with remarkable tilting of the tetrahedral chains. The value of the displacement parameters follows the trend $U_{eq}M2 > U_{eq}O2 > U_{eq}O3 > U_{eq}O1 > U_{eq}M1 \approx U_{eq}T$ for all samples belonging to the jadeite–aegirine join and for pure hedenbergite; in contrast,, for pyroxenes with intermediate compositions between hedenbergite and jadeite the trend is $U_{eq}O1 > U_{eq}O2 > U_{eq}M2 > U_{eq}O3 > U_{eq}M1 \approx U_{eq}T$, with O1 and O2 having anomalously large displacement parameters, probably due to different local structural configuration around the cations with different size and charge.

Cation substitution at the M1 site of Na-pyroxenes gives rise to a different structural deformation with respect of the double substitution at both the M1 and M2 sites in $(Na,Ca)(M^{3+},M^{2+})Si_2O_6$ pyroxenes as the rigid tetrahedral chains try to accommodate both the increasing size of the M1 site and the different coordination requirement of the M2 site.

Keywords: Single crystal, X-ray diffraction, crystal-structure, clinopyroxenes