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 (Jd74Hd26, Jd100) and jadeite–aegirine (Jd100Ae0, Jd76Ae24, Jd35Ae65, Jd0Ae100) joins were refined by means of single-crystal X-ray diffraction (space group C2/c, R_{w} 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 \(U_{eqM1} > U_{eqO2} > U_{eqO3} > U_{eqO1} > U_{eqM2} \approx U_{eqT} \) 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 \(U_{eqM1} > U_{eqO1} > U_{eqO2} > U_{eqM2} \approx U_{eqO3} > U_{eqM1} \approx U_{eqT} \), 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 \((Na, Ca)(M^{+}, M^{2+})Si_{2}O_{6}\) 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

INTRODUCTION

Pyroxenes are among the most common minerals in the crust and the upper mantle and are major constituents in several meteorites; knowledge of their structural and thermodynamic properties is hence important in petrological modeling. In particular, Na-bearing pyroxenes are key phases in high-pressure and extreme pressure assemblages, up to more than 20 GPa and 1600 °C (Tutti et al. 2000). Natural Na-bearing pyroxenes are solid solutions of jadeite (Jd, NaAlSi2O6) with aegirine (Ae, NaFe3+Si2O6), diopside (Di, CaMgSi2O6), and hedenbergite (Hd, CaFe2+Si2O6). The end-members display NaFe3+Si2O6), diopside (Di, CaMgSi2O6), and hedenbergite (Hd, CaFe2+Si2O6) end-member behavior at a short-range scale is averaged in single structure determinations of both pyroxenes along the aegirine–hedenbergite and jadeite–aegirine joins. Structural data obtained from single-crystal X-ray diffraction are limited to the end-members (Cameron et al. 1973; Rossi et al. 1983; Boffa Ballaran et al. 1998; Heuer et al. 2005; Redhammer et al. 2000), whereas refinements of both single-crystal and powder data are available for several synthetic pyroxenes along the aegirine–hedenbergite join (Redhammer et al. 2000, 2006). For the aegirine–jadeite solid solution only unit-cell parameters are reported (Liu and Bohlen 1995; Nestola et al. 2006).

Direct information on samples with mixed compositions instead of just a mere comparison between the end-members has the following advantages: (1) Cation substitution seldom occurs with fully ideal behavior. Clustering of likely cations and order-disorder behavior may occur in intermediate samples, affecting structural and thermodynamic properties. Local structural behavior at a short-range scale is averaged in single structure investigation, but may be revealed by the presence of anomalous atomic displacement parameters in the average structure for intermediate compositions (e.g., Tribaudino and Nestola 2002). (2) The structural analysis along a given join clarifies the mechanism of cation substitution. Moreover, subtle structural changes, which could be overlooked analyzing only the end-members, can be enhanced by the analysis of high quality structural data for intermediate compositions.

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