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LETTER

Crystal-structure refinement of Na-bearing clinopyroxenes from mantle-derived eclogite xenoliths

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ABSTRACT

Nine omphacitic clinopyroxenes with a jadeitic content between 25% and 57% from the Udachnaya and Zagadochnaya diamond-bearing kimberlites were investigated using single-crystal X-ray diffraction, electron microprobe analysis, and Mössbauer and infrared spectroscopy. Crystal-structure refinements, incorporating constraints from chemical analyses and Mössbauer data, show a significant concentration of vacancies at the M2 site in three of the samples. The cell volumes of the non-stoichiometric samples plot below the linear trend defined by stoichiometric diopside-jadeite compositions, where the deviation from the linear trend is positively correlated with the concentration of vacancies. Charge-balance appears to be achieved primarily through substitution of Al^{3+} for Mg^{2+} on the M1 site, which causes a contraction of the M1 site volume compared to stoichiometric clinopyroxenes with the same composition. Vacancies are not associated with OH^- incorporation, as the sample with the highest concentration of vacancies contains only 89 ppm (wt) H_2O. Significant hydrogen loss through iron oxidation during ascent is ruled out based on the low Fe^{3+} concentrations. H content in omphacite samples from kimberlites could provide a sensitive tool for determining f_{H_2O} during diamond formation.

Keywords: Crystal structure, omphacite, non-stoichiometry, water