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Single-crystal diffraction and transmission electron microscopy studies of "silicified" pyrochlore from Narssârssuk, Julianehaab district, Greenland

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ABSTRACT

Pyrochlore-group minerals that exhibit high Si contents are fairly common in geochemically evolved parageneses. However, the role of Si in the structure of these minerals is unclear. Different explanations have been invoked to clarify the way in which Si is incorporated in natural pyrochlores. These include the presence of impurities, the presence of Si in an amorphous or dispersed state, and its presence as an essential part of the structure.

This paper reports an integrated XREF, SEM, EMPA, and TEM study on pyrochlore samples with high SiO_2 content (up to 11.51 wt%) from Narssârssuk, Julianehaab district (Greenland). TEM observations reveal that Si-poor areas have strong and sharp diffraction peaks, whereas the Si-rich areas showed weaker spots with the diffuse diffraction halo typical of a metamict material. No evidence of crystalline phases other than pyrochlore was observed. Two single crystals having the unit-cell parameter a = 10.4200(7) and 10.3738(7) Å, respectively, were analyzed by X-ray diffraction and the structure was refined to R_{obs} = 2.62 and 4.35%. On the basis of both the refined site scattering and the octahedral bond distance and the results of the TEM investigation, only a fraction (~30–50%) of the Si detected by EMPA is incorporated in the structure. A comparison with structural data of Si-free pyrochlores reported in the literature supports this assumption and allows a linear multiple regression to model the effect of the substitution of (Nb,Ta) by Ti and Si. The remaining 50–70% of the total silicon detected is incorporated in the radiation-damaged portions of pyrochlore.

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