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Structure refinement of a synthetic knorringite, $Mg_3(Cr_{0.8}Mg_{0.1}Si_{0.1})_2(SiO_4)_3$

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Abstract

The crystal structure of a polycrystalline knorringite, $Mg_3(Cr_{0.8}Mg_{0.1}Si_{0.1})_2(SiO_4)_3$, synthesized at 11 GPa and $T = 1500$ °C in a multi-anvil press, has been refined from high-resolution synchrotron X-ray powder diffraction data. The structure is cubic, space group $Ia\bar{3}d$, $a = 11.5935(1)$ Å, $V = 1558.27(4)$ Å^3, $D_{calc} = 3.79$ g/cm^3. The structural formula indicates that knorringite is susceptible to majorite substitution at these synthesis conditions. The Cr-O distance, 1.959(7) Å, is similar to that in Cr-bearing pyrope $Mg_3Al_2(SiO_4)_3$. This confirms that the magnitude of the Cr-O distance is not responsible for the difference in crystal field splitting values between green knorringite and red Cr-pyrope. A comparison with the structure of other Cr-garnet end-members shows that the Cr-O distance and the $^{[4]}$Si-O-Cr angle decrease with decreasing synthesis pressure and with increasing X-cation size.

Keywords: Structure refinement, knorringite, XRD, synchrotron powder diffraction, Cr-garnet