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Khmaralite, a new beryllium-bearing mineral related to sapphirine: A superstructure resulting from partial ordering of Be, Al, and Si on tetrahedral sites

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ABSTRACT

Khmaralite, $Ca_{0.04}Mg_{5.46}Fe^{3+}_{0.12}Fe^{2+}_{1.87}Al_{14.26}Be_{1.43}B_{0.02}Si_{4.80}O_{40}$, is a new mineral closely related to sapphirine from Khmara Bay, Enderby Land, Antarctica. It occurs in a pegmatite metamorphosed at $T \geq 820$ °C, $P \geq 10$ kbar. The minerals surinamite, musgravite, and sillimanite associated with khmaralite at Casey Bay saturate it in BeO, and thus its BeO content could be close to the maximum possible. Optically, khmaralite is biaxial (–); at $\lambda = 589$ nm, $\alpha = 1.725(2)$, $\beta = 1.740(2)$, $\gamma = 1.741(2)$, $2V_{meas}$ = 34.4 (1.8)°, v > r strong, and $\beta \parallel b$. The weak superstructure reported using electron diffraction has been confirmed by single-crystal X-ray diffraction. The superstructure corresponds to a doubling of the **a** axis in monoclinic sapphirine-2*M* ($P2_1/c$ setting) with the following unit-cell parameters: a = 19.800(1), b = 14.371(1), c = 11.254(1) Å, β = 125.53(1)°, Z = 4, D_{calc} = 3.61 g/cm^3. Using a simplified chemical formula of $Mg_{5.46}Al_{14.28}Fe_{2.00}Si_{4.80}Be_{1.46}O_{40}$, the fully anisotropic structure refinement of all site occupancies, including Al vs. Mg and Al vs. Si on the 16 octahedral (M) and 12 tetrahedral (T) sites respectively, establishes that the 2×**a** superstructure results primarily from ordering in the doubled (T1 → T6, T7 → T12) tetrahedral chain, which is parallel to the **a** axis. The strongest contribution comes from Al-Si-Be ordering on the T2 (33-16-51%) vs. T8 (0-95-5%) and T3 (4-78-18%) vs. T9 (30-0-70%) sites. Thus, the sequence Al-Si-Al in sapphirine is replaced by the sequence Si-Be-Si in khmaralite; i.e., Be replaces Si on two sites and Si replaces Al on on four adjacent sites, resulting in an indirect replacement of Al by Be by the coupled substitution Be + Si = 2Al. The Be distribution in khmaralite and the strong preference for Be/Al mixing over Be/Si mixing appear to satisfy the bonding requirements of the bridging O atoms by minimizing the number of Be-O-Be and Be-O-Al linkages.