

Coussellite, $\text{CaNa}_3\text{AlMg}_3\text{F}_{14}$, a rhombohedral pyrochlore with 1:3 ordering in both A and B sites, from the Cleveland Mine, Tasmania, Australia

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ABSTRACT

Coussellite, $\text{CaNa}_3\text{AlMg}_3\text{F}_{14}$, from the Cleveland tin mine at Luina, western Tasmania, has a rhombohedral distortion of the cubic pyrochlore $\text{A}_2\text{B}_2\text{X}_6\text{Y}$ structure, with $a = 7.1756(1)$ Å, $\alpha = 59.867(1)^\circ$, space group $R\bar{3}m$, $Z = 1$. The corresponding hexagonal cell parameters are $a = 7.1620(1)$ Å, $c = 17.5972(3)$ Å. The crystals are multiply twinned about threefold axes of the pseudocubic cell. The structure was determined using X-ray data collected on a twinned crystal and refined to $R_{\text{obs}} = 0.027$ for 452 observed reflections with $I > 2\sigma(I)$. The structure is possibly unique among published structures of pyrochlore-like minerals in having full 1:3 ordering of Ca:Na in the A sites and Al:Mg in the B sites. Transmission electron photomicrographs show a nanodomain structure due to twinning on a scale of ~5 nm.

Keywords: Rhombohedral pyrochlore, new fluoride mineral, structure determination, 1:3 cation ordering in $\text{CaNa}_3\text{AlMg}_3\text{F}_{14}$