Structural study of Ca_2CrReO_6

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A sample of Ca_2CrReO_6 double perovskite was prepared in a polycrystalline form by using the encapsulated quartz tube method. The morphology and chemical composition of the sample was investigated by scanning electron microscopy (SEM) and EDS. The crystal structure parameters were determined by analysis of synchrotron high-resolution X-ray powder diffraction pattern and the crystal parameters were compared with results from Bond-Valence Method, predicted by the SPuDS program. The analysis indicates that the sample presents an ideal single-phase compound and a monoclinic crystal structure (space group $P2_1/n$) with $a = 5.44445(2)$; $b = 5.63957(3)$; $c = 7.77524(3)$; and $\beta = 90.18(1)^\circ$.

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