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Crystal structure of Cr-mullite

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ABSTRACT

A Rietveld refinement of Cr-doped mullite, $Cr_{0.5}Al_{3.92}Si_{1.58}O_{9.79}$, orthorhombic, space group *Pbam* [a = 7.56712(6) Å, b = 7.70909(6) Å, c = 2.90211(2) Å, V = 169.30 Å^3] revealed Cr to reside predominantly in the octahedrally coordinated M1 site. The mean M1-O distance of 1.935 Å is that expected from Al^{3+} and Cr^{3+} molar fractions obtained from the chemical analysis and structure refinement. The small displacement factors of the T* and Oc* sites indicate deficiencies in the electron densities which could be compensated by assuming additional Cr atoms. The predominant Cr incorporation into the M1 site causes an expansion of the octahedral bonds which is directly related to the observed lengthening of the c edge. The strong expansion of the long and elastic octahedral M1-Od bond in Cr-doped mullite, which would affect the a and b edges, is partly absorbed by a shortening of tetrahedral bonds.