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The crystal structure of chromian kassite from the Saranovskoye deposit, Northern Urals, Russia

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ABSTRACT

The crystal structure of kassite, ideally $Ca[Ti_2O_4(OH)_2]$, containing 2 wt% Cr_2O_3, from the Saranovskoye chromite deposit, Perm' district, Northern Urals, has been determined and refined to $R1 = 0.06$ using single crystal X-ray diffraction data. The crystals have monoclinic symmetry, $P2_1/a$, with $a = 5.275(1)$, $b = 9.009$ (2), $c = 9.557$ (2) Å, $\beta = 90.43°$. A pronounced sub-structure for the mineral, conforming to space group $I2/a$, is related to the $I2/a$ structure for lucasite-(Ce), $Ce[Ti_2O_5(OH)]$. It comprises (001) layers of gibbsite-like fused hexagonal rings of edge-shared $Ti(O,OH)_6$ octahedra with the Ca atoms sandwiched between pairs of opposing rings and displaced from the center of the rings along [010]. Ordering of the protons in chromian kassite lowers the symmetry to $P2_1/a$. Kassite, $CaTi_2O_4(OH)_2$, and cafetite, $CaTi_2O_5(H_2O)$, are identical chemically but significantly different in their crystal structures.