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Cafetite, $Ca[Ti_2O_5](H_2O)$: Crystal structure and revision of chemical formula

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ABSTRACT

The crystal structure of cafetite, ideally $Ca[Ti_2O_5](H_2O)$, (monoclinic, $P2_1/n$, $a = 4.9436(15)$, $b = 12.109(4)$, $c = 15.911(5)$ Å, $\beta = 98.937(5)°$, $V = 940.9(5)$ Å^3, $Z = 8$) has been solved by direct methods and refined to $R_1 = 0.057$ using X-ray diffraction data collected from a crystal pseudo-merohedrally twinned on (001). There are four symmetrically independent Ti cations; each is octahedrally coordinated by six O atoms. The coordination polyhedra around the Ti cations are strongly distorted with individual Ti-O bond lengths ranging from 1.743 to 2.223 Å (the average <Ti-O> bond length is 1.98 Å). Two symmetrically independent Ca cations are coordinated by six and eight anions for Ca1 and Ca2, respectively. The structure is based on $[Ti_2O_5]$ sheets of TiO_6 octahedra parallel to (001). The Ca atoms and H_2O groups are located between the sheets and link them into a three-dimensional structure. The structural formula of cafetite confirmed by electron microprobe analysis is $Ca[Ti_2O_5](H_2O)$, in contrast to the formula $(Ca,Mg)(Fe,Al)_2Ti_4O_{12}\cdot 4H_2O$ suggested by Kukharenko et al. (1959). The wrong chemical formula suggested for cafetite by Kukharenko et al. (1959) is probably due to admixtures of magnetite or titanomagnetite in their samples. Cafetite is chemically related to kassite, $CaTi_2O_4(OH)_2$, but differs from it in structure and structural formula.