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$Na_2Ca_2(P_2O_7)F_2$, the first diphosphate of the cuspidine family

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ABSTRACT

The crystal structure of synthetic $Na_2Ca_2(P_2O_7)F_2$ was solved from single crystal X-ray diffraction data and refined to $R = 4.31\%$ for 1234 independent reflections [$I>2\sigma(I)$]. The compound is monoclinic with space group symmetry $P2_1/n$, $a = 10.8730(21)$ Å, $b = 10.5516(25)$ Å, $c = 7.4287(13)$ Å, and $\beta = 109.74(2)°$ and twinned by pseudo-merohedry with $m_{(100)}$ as the plane of twinning which was accounted for in the refinement calculations. The crystal belongs to the structure family of the mineral cuspidine and represents the first phosphate member of this group. The structure is characterized by ribbons of four MX_6-octahedra (M = Na,Ca; X = O,F) running parallel to **c**. Within a single ribbon the octahedra are linked by edge-sharing, whereas two adjacent ribbons are connected via common corners. Further linkage results from the diphosphate groups, sharing each of the six equatorial oxygen atoms with adjacent octahedral ribbons. Using the modular description usually applied for the classification of cuspidine type structures the present compound belongs to the so called type 5 and is the first representative of this class.