The Crystal Structure of the Potential Ferroelectric Calcium Rhenate(VI, VII) $Ca_{11}Re_4O_{24}$ and its Relation to the Structure of $Sr_{11}Os_4O_{24}$

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Z. Naturforsch. **53 b,** 31–36 (1998); received October 17, 1997

Crystal Structure, Ferroelectrics, Mixed Valence, Rhenates, Perrhenates

The title compound was prepared in well-crystallized form by thermal decomposition of $Ca_5Re_2O_{12}$. Its structure was determined from single-crystal X-ray diffractometer data: $I4_1$, a = 1107.0(1), c = 1609.3(1) pm, Z = 4, R = 0.056 for 4565 structure factors and 119 variable parameters. The calcium atoms occupy seven different sites with 8, 9, or 10 oxygen neighbors. The two different rhenium atoms are octahedrally coordinated by oxygen atoms with average Re-O distances of 193.1 and 187.7 pm for the six- and seven-valent rhenium atoms, respectively. The compound shows Curie-Weiss behavior with a magnetic moment of μ_{exp} = 1.15(±0.10) μ_B per Re(VI) atom. The structure is closely related to that of $Sr_{11}Os_4O_{24}$ which, however, crystallizes in the space group $I2/a$. The difference between the two structures arises through the higher coordination numbers of the strontium atoms. It is suggested that at high temperature both compounds crystallize in the common higher symmetry space group $I4_1/a$. Since $Ca_{11}Re_4O_{24}$ crystallizes in the pyroelectric class 4 this compound is expected to be ferroelectric.

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