Low Temperature Crystal Growth and Structure of Ordered $Ba_7F_{12}Cl_2$

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Crystals of composition $Ba_7F_{12}Cl_2$ were obtained by a reaction at room temperature between $Ba^{2+}/Cl^-/F^-$ in a gel of agar-agar/water. The hexagonal crystals have space group $P\bar{6}$, a=1064.69(8), c=417.89(5)pm, V=410.24(8) 10^6 pm^3 and Z=1. The anions form a propeller type network located in tunnels parallel to the c_{hex} axis; the chloride ions are located at the center on the propeller axes. The Ba^{2+} ions are coordinated by a (distorted) tricapped trigonal environment of fluoride and chloride anions. Disorder is present for one particular Ba^{2+} site. The average structure is isotypic with the structure of $Pb_7F_{12}Cl_2$.

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