Bariumfluorochloride, Hexagonal Crystal Structure, Crystal Growth, Low Temperature Gel Method

Crystals of composition Ba$_7$F$_{12}$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 P6, $a=1064.69(8)$, $c=417.89(5)$ 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 $c_{\text{hex}}$ 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$_7$F$_{12}$Cl$_2$.

* Reprint requests to Prof. H. Bill.