Poster

Which one is the right space group?

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Finding the right space group for a crystal structure is always a crucial step in structure solution. But sometimes, it can indeed cause a great difficulty for the crystallographer especially in the case of inorganic compounds with high crystal symmetry. High symmetry, supercell structures, crystal mosaicity, twinning and disorder all can make the determination of the space group difficult.

Diamminesilver(I) selenate crystallizes in the tetragonal crystal system with unit cell parameters $a = b = 8.5581(1)$ Ä, $c = 6.5187(1)$ Å, $\alpha = \beta = \gamma = 90°$. The structure can be solved in both $P\text{-}42_1c$ and $I4/mmm$ space groups with R_1 values 2.40 % and 2.23 % respectively. In the high-symmetry space group, both the diamminesilver(I) complex and the selenate ions are disordered.

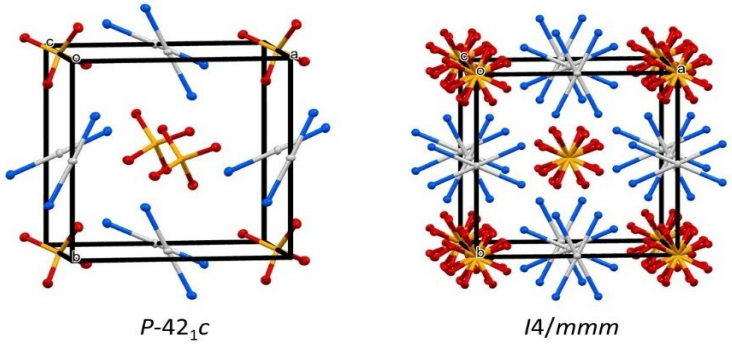

Figure 1. Unit cell of diamminesilver(I) selenate with different space group symmetries

The crystal structure of potassium hexamminecobalt(III) dichloride dipermanganate is $R\text{-}3m$ trigonal at -170 °C ($a = b = 6.9642(8)$ Å, $c = 27.6254(9)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$). At 0 °C, it can be solved in both the $C2/m$ monoclinic (a = 12.2264(9) Å, b = 6.9946(5) Å, c = 12.2825(8) Å, $\alpha = \gamma = 90°$, $\beta = 131.127(9)°$) and the $R\text{-}3m$ trigonal ($a = b = 6.9942(3)$ Å, $c = 27.7569(9)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$) space groups with similar R_1 values. The atomic arrangements are similar for the two different unit cells.

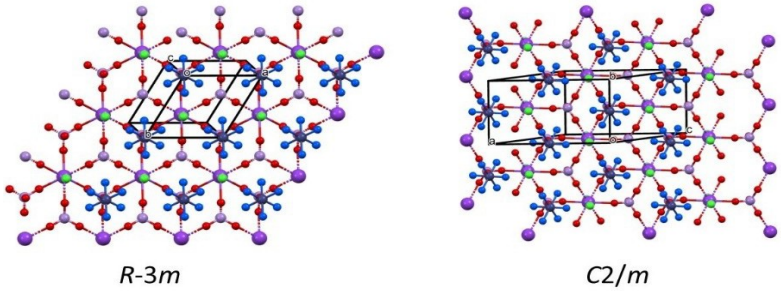

Figure 2. Crystal structure of potassium hexamminecobalt(III) dichloride dipermanganate with different unit cells

For both compounds, there are indirect indications for the existence of polymorphic phases on the basis of thermoanalytical data.