

Space group of diglycine barium chloride monohydrate

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Diglycine barium chloride monohydrate crystallizes in the orthorhombic system with a tetra-molecular unit cell, the dimensions of which, determined from rotation and equi-inclination Weissenberg photographs, are

$$a = 8.302 \pm 0.015 \text{ \AA}, \quad b = 14.801 \pm 0.025 \text{ \AA}, \quad c = 9.324 \pm 0.015 \text{ \AA}; \\ Z = 4.$$

The density was measured by the flotation method using α bromoform and carbon tetrachloride. ρ measured = 2.2 g/cm³, ρ calculated = 2.182 g/cm³.

The extinctions are:

$$\begin{array}{ll} hk0 \text{ with } h+k = 2n+1 & h00 \text{ with } h = 2n+1 \\ 0kl \text{ with } k = 2n+1 & 00l \text{ with } l = 2n+1 \\ h0l \text{ with } l = 2n+1. \end{array}$$

Hence the space group could be uniquely fixed to be the centrosymmetric space group $Pbcn (V_h^{14})$.

The principal refractive indices of the crystals were measured for $\lambda = 589 \text{ m}\mu$ at 32°C with immersion media of nitrobenzene and α bromonaphthalene. The crystals are biaxial and optically negative with $n_\alpha = 1.53990$, $n_\beta = 1.59554$, $n_\gamma = 1.60225$, $2V = 47^\circ$.

Note added in proof. The crystal structure has now been solved by the heavy-atom method. Refinement of the coordinates from three-dimensional data is under progress.