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

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

The density was measured by the flotation method using 1X bromoform and carbon tetrachloride. \( \rho \) measured = 2.2 g/cm\(^3\), \( \rho \) calculated = 2.182 g/cm\(^3\).

The extinctions are:

- \( h00 \) with \( h = 2n + 1 \)
- \( 0k0 \) with \( k = 2n + 1 \)
- \( h0l \) with \( l = 2n + 1 \)
- \( 00l \) with \( l = 2n + 1 \)

Hence the space group could be uniquely fixed to be the centrosymmetric space group \( Pbcn (V^4) \).

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

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.