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LETTER

Crystal structure of abelsonite, the only known crystalline geoporphyrin

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ABSTRACT

The crystal structure of the unique nickel porphyrin mineral abelsonite, $NiC_{31}H_{32}N_4$, has been solved using direct methods with 2195 independent reflections to a final $R_1 = 0.0406$. Abelsonite crystallizes in the triclinic space group $P\bar{1}$, with $Z = 1$ and unit-cell parameters $a = 8.4416(5)$ Å, $b = 10.8919(7)$ Å, $c = 7.2749(4)$ Å, $\alpha = 90.465(2)°$, $\beta = 113.158(2)°$, and $\gamma = 78.080(2)°$ at the measurement condition of 100 K, in very good agreement with previous unit-cell parameters reported from powder diffraction. The structure consists of nearly planar, covalently bonded porphyrin molecules stacked approximately parallel to $(1\bar{1}1)$, and held together by weak intermolecular Van der Waals forces. The molecules within a layer are slightly tilted such that molecular planes do not overlap, and an up-turned ethyl group on one molecule sits adjacent to a down-turned ethyl group on a neighboring molecule of the same layer. Layers are stacked along a vector normal to $(1\bar{1}1)$ such that an aromatic ring at one corner of the molecule lies directly above the opposite aromatic ring of the molecule below. Although a single molecule does not quite possess $\bar{1}$ symmetry, matching ethyl groups at roughly opposite ends of the molecule enable orientational disorder, in which molecules can randomly adopt one of two different orientations while still stacking in the same manner. The aggregate of these two random orientations produces an overall symmetry of $P\bar{1}$.

Keywords: Abelsonite, crystal structure, porphyrin, geoporphyrin, organic, orientational disorder