

Abstract Submitted  
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**'Guanigma': the revised structure of biogenic anhydrous guanine** ANNA HIRSCH, DVIR GUR, Weizmann Institute of Science, Israel, IRYNA POLISHCHUK, DAVIDE LEVY, BOAZ POKROY, Technion, Israel, AURORA J. CRUZ-CABEZA, University of Manchester, United Kingdom, LIA ADDADI, LEEOR KRONIK, LESLIE LEISEROWITZ, Weizmann Institute of Science, Israel — Living organisms display a spectrum of colors, produced by pigmentation, structural coloration, or both. A relatively well-studied system, which produces colors via an array of alternating anhydrous guanine crystals and cytoplasm, is responsible for the metallic luster of many fish. The structure of biogenic anhydrous guanine was believed to be the same as that of the synthetic one - a monoclinic polymorph. Here we re-examine the structure of biogenic guanine, using experimental X-ray and electron diffraction (ED) data exposing troublesome inconsistencies - namely, a 'guanigma'. To address this, we sought alternative candidate polymorphs using symmetry and packing considerations, then used first principles calculations to determine whether the selected candidates could be energetically stable. We identified theoretically a different monoclinic polymorph, were able to synthesize it, and to confirm using X-ray diffraction that it is this polymorph that occurs in biogenic samples. However, the ED data were still not consistent with this polymorph, but rather with a theoretically generated orthorhombic polymorph. This apparent inconsistency was resolved by showing how the ED pattern could be affected by crystal structural faults composed of offset molecular layers.

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