

ELDICO ED-1 Unveils Groundbreaking Advancements in Biogenic Crystal Structure Determination with 3D Electron Diffraction!

Biogenic material

Biogenic crystals are crystals produced by living organisms, such as calcium oxalate crystals found in various plant tissues, magnetite crystals forming within diverse bacteria and animals, and various crystals appearing in the human body. These crystals are a subject of considerable interest due to their captivating and unique properties.

The susceptibility to undergo damage upon extraction from the parent organism presents major challenges to structure determination of biogenic molecular crystals. The size range spanning from nanometers to micrometers, poses challenges for determining their structures using traditional methods like single-crystal X-ray diffraction (SC-XRD) or powder X-ray diffraction (PXRD).

Electron diffraction

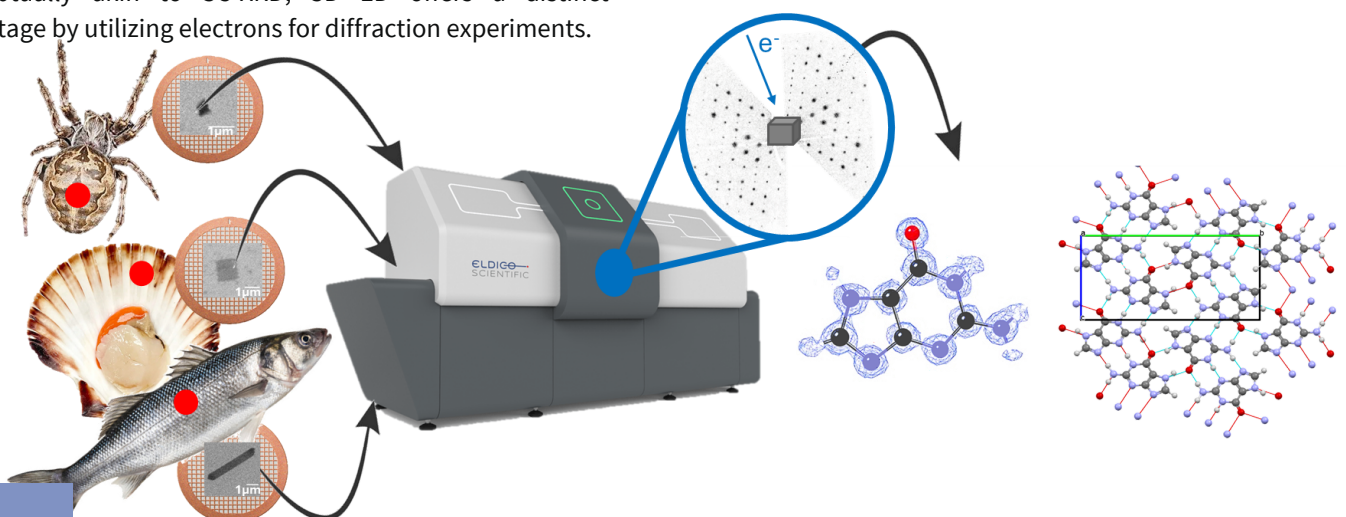
3D electron diffraction (3D ED) methods, also known as microcrystal electron diffraction (microED), have experienced rapid advancement in recent years. Although conceptually akin to SC-XRD, 3D ED offers a distinct advantage by utilizing electrons for diffraction experiments.

Thanks to the strong interaction between electrons and matter, 3D ED data can be collected from crystals with volumes 10^6 times smaller than those required for X-ray diffraction, even when coexisting in mixture. Thus, crystals from what traditionally would have been considered as powder samples by x-ray standards can now be handled as single crystals by electron diffraction.

ELDICO ED-1

The ELDICO ED-1, the worlds first dedicated electron diffractometer, has been designed to measure crystallites in the nanometer range under ambient or cryogenic conditions.

It is designed to collect data with the minimal electron exposure of $<0.01 \text{ e-}/\text{\AA}^2/\text{s}$, by illuminating small area during data collection. This makes it optimal for data collection from beam sensitive materials like organic crystals.



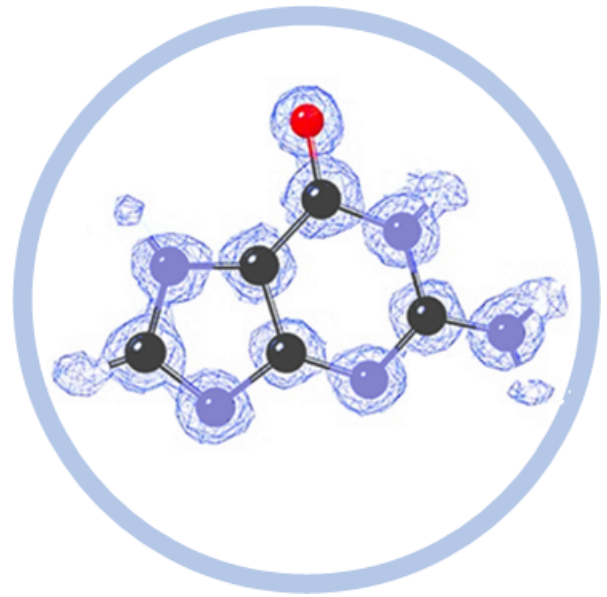
Case study: Guanine crystals in spider integument, fish scales and scallop eyes.

In collaboration with scientists from Ben-Gurion University of the Negev, Cardiff University, and our application science team from ELDICO Scientific AG we analyzed biogenic crystals extracted from fish scales, spider integument, and scallop eyes.

Results

Table 1: Details of the refinement of the structure of the β -polymorph of guanine [1]

Sample	Fish	Spider	Scallop
Resolution [\AA]	0.67	0.67	0.80
Reflections	5155	6019	2289
Completeness [%]	87.4	97.7	80.2
R1 [all refl.]	0.195	0.278	0.446
R1 [$I > 2\sigma(I)$] [%]	0.177	0.241	0.374
wR2 [all data]	0.537	0.540	0.735
Goodness of fit	2.425	2.027	3.006

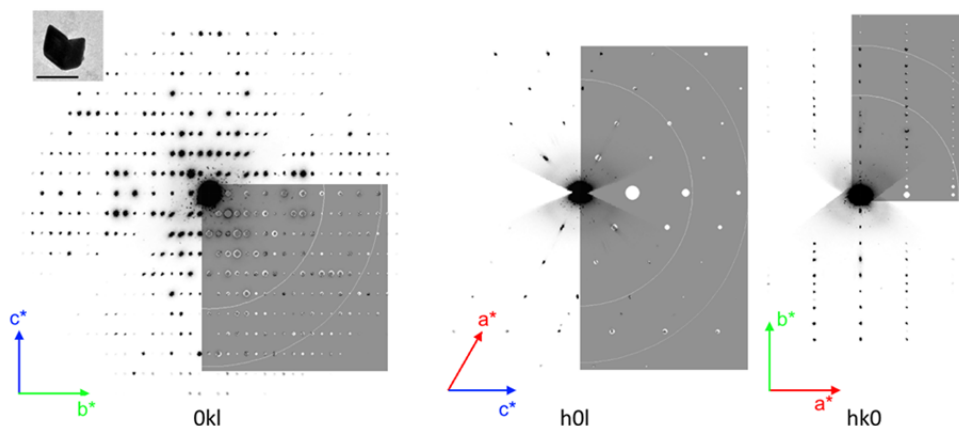


The hydrogen atoms were located directly in our structure determinations from 3D ED data, representing an improvement in the quality of the β -guanine crystal structure compared to the structure published previously

Conclusion

The findings represent a crucial step forward in understanding and harnessing the potential of biogenic crystals for sustainable and bio-compatible optical applications. Key benefits of the ELDICO ED-1 are:

- effortless data collection
- ab initio structure solution
- refinement of the structures free of restraints
- no need of pure compound, data collection directly from crude material
- accurate electrostatic potential map from which hydrogen atoms could be directly located



With the ELDICO ED-1 the experimental diffraction data show a perfect match with the simulated data

[1] Hirsch, A.; Gur, D.; Polishchuk, I.; Levy, D.; Pokroy, B.; Cruz-Cabeza, A. J.; Addadi, L.; Kronik, L.; Leiserowitz, L. "Guanigma": The Revised Structure of Biogenic Anhydrous Guanine. *Chem. Mater.* **2015**, 27 (24), 8289–8297

