ELDICO SCIENTIFIC
THE ELECTRON DIFFRACTION COMPANY

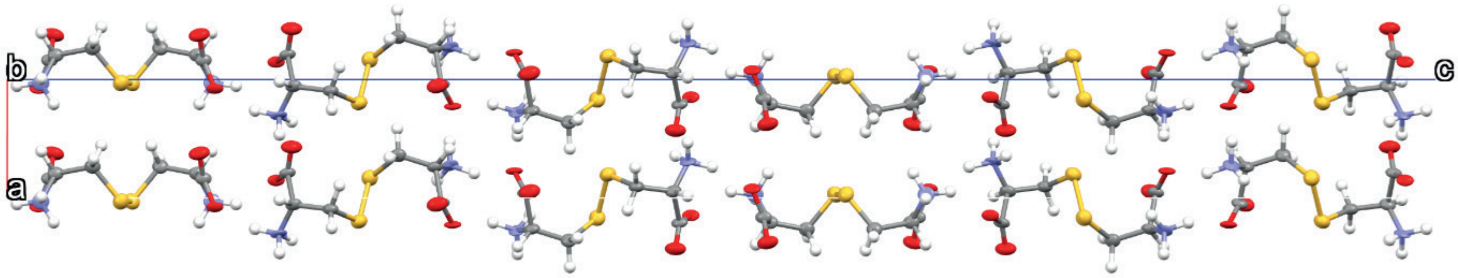
Long unit cell axes: *ED-1* CAN HANDLE "BIGGER" PROBLEMS

ELDICO ED-1: Advantages of it's simplified Optical design for crystallographic challenges

There are only few examples of small molecules crystallising in unit cells with cell axes longer than 50 Å. The potential of *ELDICO ED-1* to perform structure elucidation of structures with long unit cell axes has been shown of the example of Cystine ($C_6H_{12}N_2O_4S_2$). Cystine crystallises in a hexagonal unit cell with a c axis of 56.8 Å and is perfectly suitable for a test of how the device performs with long cell axes.[1]

ELDICO ED-1 captivates with a simplified design featuring no optics between the detector and the sample stage resulting in largely reduced distortion of diffraction pattern. The fixed detector length for the *ELDICO ED-1* is one reason for the simple and reliable unit cell determination without further processing of the raw image files. On this example we show that the fixed detector length is no hinderance for an accurate spot identification and integration process of structures with bigger cell axes.
Data processing was performed using the APEX4 software package and implemented programs. With angles of α = 89.90°, β = 90.04° and γ = 120.03° for the unrestricted unit cell and standard uncertainties of less than 0.5 % for the cell axes of the restricted unit cell, the unit cell determination is as good as usual for datasets measured with the *ELDICO ED-1*.

Due to the preferred orientation of the small plate-like crystals several datasets were merged to reach the necessary completeness for a structure solution using SHELXD. H atoms were placed in calculated positions. All protons of the R-NH_3+ group can be found from the difference Fourier maps, showing the good quality of the refined structure solution.



[1] B. M. Oughton & P. M. Harrison, *Acta Cryst.* **1959,** *12*, 396.

Electron diffraction — pushing the boundaries of crystallography

As every crystallographer knows: Crystallization is a tricky thing. Obtaining crystals large enough for X-ray diffraction experiments is not that easy. In many cases, it isnt even possible. And there is more: Only electron diffraction can provide the fastest and most convenient access to a variety of analytical approaches that will shape the future of crystallography.

Electron diffraction supports sophisticated research challenges such as

- Nano-crystals
- Location of light elements
- Detection of mixtures and impurities

The challenge

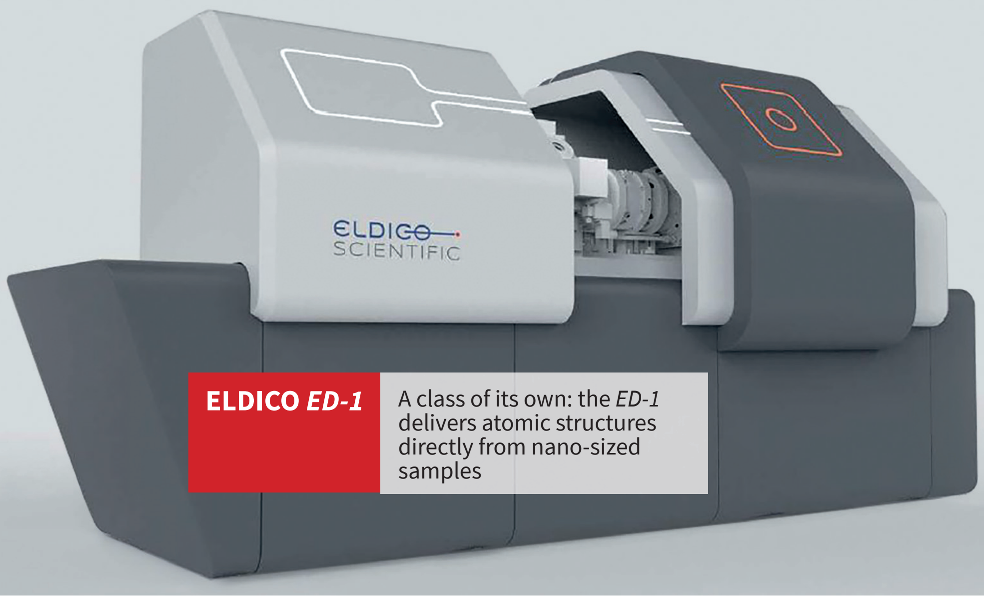
Growing crystals large enough for the X-ray experiments can take weeks, months or even years. This proves to be a true bottleneck for crystallographic experiments at nano-scale.

The solution

Electron diffraction is the method of choice to elucidate structures as small as 50 to 500 nanometers, directly from the flask.

APPLICATIONS FOR ELECTRON DIFFRACTION

1. Structure **ELUCIDATION**
2. Assist **CRYSTAL STRUCTURE PREDICTION**
3. Impurity **IDENTIFICATION**
4. Crystal mapping: **MICRO CRYSTALLINITY OF AMORPHOUS SOLID DISPERSIONS**
5. Absolute **STRUCTURE DETERMINATION**
6. Identification of **UNKNOWN PHASES**
7. Quality **CONTROL**



ELDICO *ED-1* A class of its own: the *ED-1* delivers atomic structures directly from nano-sized samples

The need for a dedicated device for electron diffraction is evident. ELDICO *ED-1*, the first dedicated electron diffractometer and as such a class of its own, has been designed to measure samples of solid compounds in the nanometer range under ambient or cryogenic conditions (optional). It is targeted to achieve resolution of up to 0.84 Å, in the majority of cases, with at least 60-70% complete datasets. Unit cell determination can be as accurate as 1:1,000.

- **ELDICO *ED-1* – rapid data collection under ambient or cryogenic conditions**
- **Superior performance for advanced crystallographic applications**

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