

MS45. Chemical information as prior knowledge in crystallography

Chairs: Anthony Linden, Rob Nicholls

MS45-P1 X-ray origins: protection or paranoia?

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Deliberate fabrication of crystallographic data has previously led to falsified structures being published and then later retracted from respected scientific journals¹⁻³. Identified perpetrators, in these cases, had made very simple modifications to structural files, such as manually changing unit cell sizes and atom types, to produce adjusted data. Fortunately they were found to be unable to produce raw experimental data to support their claims. Kroon-Batenburg and Helliwell⁴ proposed that the requirement for the deposition of raw crystallographic data may be a potential method of preventing the submission of counterfeit structures. However we can show that the recreation of raw diffraction images is no longer difficult, opening the doors for those less scrupulous to take advantage, if this is not already occurring!

Detector frame formats from many manufacturers are well documented and this information can be reverse-engineered to encode synthetic diffraction data. This process was brought to light as a product of research into optimising data collection parameters for charge density studies. The chosen method required us to produce an algorithm which takes data from integrated *.raw* files as a starting point to create replicas of experimental images. A simple misuse of this code could take structure factors calculated for an entirely fabricated compound and produce diffraction images that, when processed, return the artificial structure. The frames are not visually distinguishable from authentic, experimentally determined, ones and can be fully integrated using standard protocols. The authors find this situation potentially alarming and requiring immediate attention.

A structure refined from data processed from these artificial diffraction images pass all IUCr checkCIF⁵ protocols without raising alerts. We will present such a structure, full details of the algorithms employed and propose methodologies that may safeguard against this approach going undetected.

References

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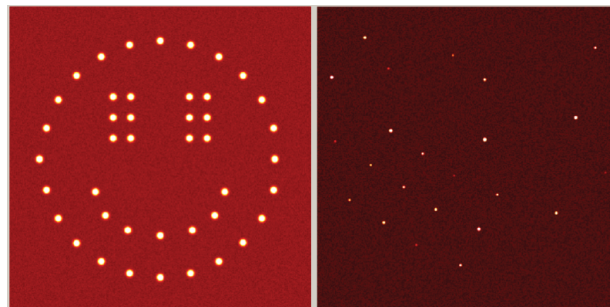


Figure 1. Two diffraction images - which is real?

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