

Can We Trust Structures from Powder Diffraction Data?

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Powder diffraction is a long-accepted technique for identifying and quantifying crystalline materials. Since the introduction of the Rietveld method of profile analysis, powder data is increasingly used for solution and refinement of crystal structures. The past 20 years have seen a dramatic growth in the number of crystal structures solved on the basis of powder diffraction measurements, although it is still a tiny fraction of the total. There is clearly less information in a typical powder diffraction pattern than in a typical dataset from single crystal measurements, and those publishing structures based on powder data are a small minority of the active crystallographic community. Since many scientists seem to be dubious about the veracity of structures from powder data, the title of this talk is a natural question. There is no simple, general answer.

One can get some insight into the issues by looking at cases where a structure was published from a powder sample and subsequently, or at least independently, from a single crystal. I will review a limited set of examples.

I will share some informative incorrect structures, point out some pitfalls, and propose that the answer to this dilemma is social, not technical. To wit:

- For every publication of a structure from powder diffraction, the raw data and computed profile should be deposited where it will be publicly accessible.
- All journals should seek the counsel of those familiar with powder crystallography in reviewing manuscripts for publication.

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