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Editorial

# Reviewing Crystallographic Data—Sifting CIFs

Nearly forty years ago as a summer student at Brookhaven, I performed my first crystal structure determination. It was a stimulating and intimidating initiation to research. One week for crystal alignment, three weeks of multiple film Weissenberg photographs, three more weeks of visually estimating intensities (nearly 10000 "spots" by the end of the summer), punched cards for the intensity data (I was relieved of that exercise), and then boxes and boxes of cards and days and days of batch jobs for Fourier maps and least squares refinements, followed by final error analysis and building a cork-ball model (ORTEP was still one or two years in the future). Overall, three months, two structures, a pair of glasses and three-foot-high stacks of computer output. I came away from that summer committed to the value of X-ray crystallography for inorganic chemistry and dazzled by the amount of data generated. Jim Ibers was a tough taskmaster and a good teacher in rigorously checking the tables submitted for publication, including $F_o - F_c$ or structure factor tables.

Fast forward to the present. With new CCD instrumentation and associated computer hardware and software, it now takes 12 hours to accomplish what I did in three months. X-ray crystallography is now more important than ever, and its use in characterizing inorganic systems is growing at a mind-numbing clip. Approximately 70% of the submissions to *Inorganic Chemistry* have at least one crystal structure, and many have more. Each CCD structure generates many megabytes of data (if one saves the raw frames) compared to my boxes of punched cards processed on an IBM 7094 with a staggering 64K of memory. Today's structure solution packages are superb, and it is not unusual to "solve and refine" a structure successfully (though possibly not optimally) by doing nothing more challenging than hitting the return key. This should be cause for rejoicing. And it is. But it is also a cause for concern.

As we do more crystallography, do we know more about it—or less? Do we check ourselves and the data more—or less? Do we check the papers we review for crystallographic content more—or less? Do we access the crystallographic information files (CIFs) that others submit? There is, of course, the associated question, Should we? Why not have a crystallographic guru check what others submit in the way of structural data? Actually, with the current volume of structural studies, in order to do this right, we would need several. How much is our responsibility as scientists, researchers, authors and reviewers to know the fundamentals and particulars of a particular method we routinely use and whose results form the basis of much that we analyze?

The topic of Supporting Information for crystallographic studies has been a subject of long-standing discussion. In 2001, we adopted a policy that served to reduce the amount of hard-copy data submitted with each paper and facilitate the deposition of Supporting Information electronically. The policy requires CIFs to be submitted electronically (e-mail or disk) at the time of manuscript submission with no need for submission of Supporting Information tables in hard copy or paper form. The change in policy has made it easier for authors reporting structural results. Feedback has in general been positive. The CIFs are available for reviewers at http://pubs.acs.org/reviewcif/index.html, and once a paper is published they are accessible at http://pubs.acs.org.

While this policy regarding X-ray data facilitates the submission process, it raises questions about how effectively crystallographic data are now reviewed. Are reviewers routinely accessing CIFs for the papers they are reviewing? Is it the responsibility of the inorganic chemistry community to have a high level of understanding of a method that we use so extensively? Is it our responsibility to teach students this method in a way that demands real comprehension rather than just simple navigation through the data collection and refinement software? I hope the answers to these questions are obvious—and affirmative.

In order to gain a better understanding of the current situation with regard to the review of crystallographic data, I have organized a simple survey that I hope you will fill out and return when you are asked to review a paper. You need only fill the survey out *once.* I also invite your comments on this important issue of the review of crystallographic data in *Inorganic Chemistry.* You can e-mail me at inorg@chem.rochester.edu. I plan a follow-up editorial to provide you with survey results and to share some of your comments with the entire *IC* community.

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