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book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.

Structure Determination by X-ray Crystallography. By Mark Ladd and Rex Palmer. Pp. xlii + 819. New York: Kluwer Academic/Plenum Publishers, 4th ed., 2003. Price (paperback) GBP 41. ISBN 0-306-47454-9.

It was a daunting task to take on this book review which is more like commenting on an institution *i.e.* the label that surely is required when a book reaches its fourth edition. Evidently the book, *via* its three previous editions, has acquired a strong following and must have *de facto* 'sold out'. The authors' preface to this edition opens with the statement 'There have been many advances in X-ray crystallography since the production of the third edition of this book, and we have endeavoured to introduce a number of them into this new edition . . . In particular we have extended the discussion of the theory of X-ray diffraction and added new chapters on structure determination from powder data, on macromolecular crystallography and on computational procedures in X-ray crystallography . . . This edition is accompanied by a suite of computer programs on a compact disc. The programs are available also online . . . '. Thus briefed, and armed with my much thinner third edition I set off on my journey to review this book.

I started with a read of the Foreword by Professor Mike Glazer. I became alarmed when Mike embarked on what might be called a tirade against those he called Practising Crystallographic Idiots (PCIs). These he argued, with evidence (although inappropriately attributed to the IUCr), were those producing structures of molecules without apparently having a proper understanding of the method, and thereby having a significant probability of getting a structure wrong. The book, Ladd and Palmer, he exhorted will convert PCIs into PCEs (Practising Crystallographic Experts). On reflecting on my sense of alarm, I began to see that perhaps Mike's shock tactics made sense, *i.e.* we hardly have any (none?) crystallography departments to which undergraduates might be treated to an in-depth suite of courses on all aspects of crystallography. Rather, we have crystallography perhaps taught in a nine-lecture, or occasionally up to 18-lecture, course to biochemists, chemists or physicists. To shock the wide world of all practising crystallographic scientists that proficiency in the principles and practice of crystallography is very important, indeed vital, is the next best option for stimulating interest in learning in depth about crystallography.

In looking at the path ahead of me to evaluate these 864 pages and CD-ROM of software learning tools I had the PCI to PCE issue rather preying on my mind. Will this book succeed in this ambition? Furthermore, if one has the third edition should I recommend that one should consider buying the fourth edition?

I decided that the two new chapters on macromolecular crystallography and on powder diffraction, as well as the computational crystallography and CD-ROM aspect, required very close inspection *i.e.* being totally new as well as looking for modernization of the previously published chapters. The strengths of the new chapters lay in their full coverage of the topics. Futhermore, they linked well with the earlier chapters providing an overall unity of treatment, a major strength of this book. I read the protein crystallography chapter as a daily practitioner immersed in the subject and the powder diffraction chapter as a relative novice. I did find a few gaps of treatment in both. There was the absence of a description of the single-wavelength anomalous dispersion (SAD) technique; this is not surprising because of its rapid and recent growth since 2002. The description of the crystallization process would have benefitted from a phase diagram. The references to the heavy-atom reagents most prevalent in the MIR phasing method were old and could have been accompanied by URLs to the heavy-atom reagent databases. High-brilliance microfocus X-ray tubes are also quite recent and are missing here. More surprisingly, for a chapter carefully making a distinction between protein and macromolecular crystallography, any substantive comment about virus crystallography or structure was missing. There were also points of emphasis not to my liking; *e.g.* 'the precession camera is an invaluable tool for checking unit cell and (making) intensity checks for MIR'. Much as I admire still the ingenuity of the precession method (and spent many experiments using it myself but many years ago) I find it very difficult to believe this is true today. There was the odd mistake to keep the alert student on their toes; *e.g.* on p. 647 a molecular weight of 20 000 is stated to be 3200 C atoms *i.e.* it has been divided by 6 rather than 12. However, as a supervisor my overall feeling was that I could use this chapter (63 pages) as a good basis for teaching. This was fuelled by the full breadth of coverage and its evident strengths of its description of molecular replacement, and of protein model refinement and validation.

The powder diffraction chapter I read with less experienced eyes. I learnt from lucid descriptions of powder cameras and the powder field's preferred methods of monochromatization, of the complexities of indexing, of reflection-intensity extraction and of structure refinement from powder profiles. There then came the topic of *ab initio* structure determination and the growth of a variety of methods that have proved successful 'up to 60 atoms'. I was struck by a recurrent theme here which was the use of random approaches such as randomly placed atoms and randomly assigned phases. Here was a description of what worked but not really why it worked. One could probably assume that brute force of computer

power is the answer but I thought that more principles could have been brought to bear in this chapter.

How much updating has been done for the other chapters? This was quite a challenging job to evaluate; with the third edition to hand I made comparisons. For the contents pages I immediately found a greater, and very valuable, use of subheadings in the new edition. The side-by-side comparison of chapters revealed a substantive reordering of topics. Also the first eight chapters in this edition comprised 566 pages, the third edition had 486 pages. The order of topics looks logical except that I would have left the optical examination sections earlier in sequence, indeed much earlier on the basis that crystal growth is monitored and then followed visually before any X-ray examination takes place. I specifically looked for updating of topics where much recent work has been carried out. As good candidates I examined the authors' descriptions of Laue diffraction, MAD and neutron crystallography. For Laue diffraction in chapter 4 the explanation of how multiple reflections occurred was clear. But the finding that even with an infinite bandpass the properties of integers and of prime numbers yields a majority proportion of non-multiples was not explained. Indead the book simply states that with a 'restricted bandpass such as 0.6 to 1.6 Å the multiplicity of orders proves to be less of a difficulty than at first thought', which is also true but a supplementary point. On MAD in chapter 6 the text states that the measurements required are FP(h,k,l), $\mathrm{FPH}^{+}_{\lambda1}$, $\mathrm{FPH}^{-}_{\lambda1}$ and $\mathrm{FPH}^{+}_{\lambda2}$. But the big advantage of MAD is that FP is not needed. Also, the most popular chemical element in use for MAD is documented to be Se and yet the selenomethionine approach is not mentioned nor is Se in the list of elements found in proteins (Table 6.7). Like the Laue multiples I was again disappointed. On the third topic of most detailed checking of the updating, neutron crystallography, I was less expectant given that the title of the book is about X-rays in crystallography. The pages given to this were indeed rather few but lucidly explained. In my opinion the neutron crystallography topic is set for a big expansion, time will tell.

The above covers my journeys into the writing, but what about the software? This is the area of potential major innovation as a learning experience for students and experienced workers migrating from one crystallographic field to another. I readily loaded copies of the CD onto my laptop. The instructions carefully distinguished double clicks (DC) from single clicks (SC) and off I sailed. Firstly into the use of the *XRAY* system to solve and then refine the molecular structure of the first example, C12H14N6S2Ni (an Ni *o*-phenanthroline complex). This was one of several molecules neatly sitting basically in a plane thus affording two-dimensional calculations. The contoured native Patterson looked congested with peaks but the book helpfully steers the Ni peak picking and then also that for the sulfurs. Structure-factor calculation and difference Fourier cycling added some of the other atoms. My isotropic refinement lowered the R factor, my main feedback of progress. I could not develop this structure further as my difference Fourier was featureless for the other atoms and also I couldn't see where to input a different contour level. Instead the book tabulated the atom positions and which could be keyed in; my R factor dropped to 15%. Another review of this book has criticised the lack of data sets and indeed the convenience of the choice of two-dimensional structures. Given current PC and laptop computer power this does indeed seem unnecessary. However, the overriding sense I had here was both of fun and of providing a major teaching opportunity to a class of students. This chapter and CD alone guarantee success for this book. The powder software was equally good fun and structure solution proceeded with test solutions appearing in rapid succession from *ESPOIRE* and success monitored *via* a running best structure solution thus far. There was also a folder of general programs; the least-squares line worked and indeed is a very useful utility to make available. I tried *FOUR1D* but the page disappeared before results appeared as it did next with *MOLGOM*. The chapter had started with a statement that improved software would be available at http://www.wkap.nl/subjects/crystallography. However, this connected me with the Springer website and my attempts to find the correct icon failed; services to instructors offered complimentary copies of books but no software, media was not computer media *etc*. Perhaps worst of all the list of subjects did not contain the word crystallography, which is where this book review started. Clicking on the book title, after searching on the authors' names, revealed the book description held by the publisher; interestingly this was only held under the banner of chemistry. The website support aspects I can regard as teething problems but the authors hopefully can use the details of this review to get the web service improved.

The book could have an equally big following of the software and structure solution studies, perhaps even accompanied by a bulletin board of experiences and challenges uncovered by the students who will use the software. Indeed herein lies perhaps the best solution to getting crystallography into curricula rather than lecture courses *per se*.

In summary, this book contains a vast wealth of experience from two teachers and researchers of many years experience. I have probably asked too much in my detailed picking and unpicking; after all a lecturer should also keep on his/her toes and compare/contrast what is in a book with their own treatment and emphases of a subject. Indeed, I admired the breadth of coverage and the obvious erudition of the authors. Most important of all, and a striking feature of the book, is that it emphasises a unity to crystallography whether it be applied to biology or chemistry or materials. The book I concur is much extended over the third edition but some modernization is still required on specific topics as detailed above. As for the price of the book this is accessible, and at 864 pages including a CD-ROM, should guarantee that anyone seriously wishing to become a Practising Crystallographic Expert really should buy it and be able study hard and well with it.

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