

6. Crystal dimensions and orientation with respect to crystal axes and spindle axis; μ ; absorption correction method; maximum and minimum absorption corrections.
7. Intensity measurement:
 - (a) If film: method used to measure intensities; method of scaling intensities.
 - (b) If diffractometer: type of geometry; detector and operating conditions: derivation of integrated intensity from measurements.
 - (c) Measure of agreement among equivalent reflexions.
 - (d) Method of assigning σF_{meas} : definition of unobserved reflexions.
 - (e) Number of reflexions measured; number of independent reflexions; $(\sin \theta)/\lambda$ range within which reflexions systematically measured; total number of reflexions accessible.

III. Structure determination and refinement

1. Brief outline of method used: give details only if new methods are developed.
2. Computer programs; names and references.
3. Atomic scattering factors; ionization state assumed; source of scattering amplitudes.
4. Anomalous scattering. Values and sources of $\Delta f'$ and $\Delta f''$.
5. Extinction: coefficients and maximum percentage change in F_{meas} .

6. Weighting procedures:
 - (a) Function minimized in least-squares refinement, e.g. $\sum w(\Delta F_{\text{meas}})^2$.*
 - (b) Relation used between weights and estimated errors as assigned in II.7(d).
 - (c) Definition of R [$\sum \Delta F_{\text{meas}} / \sum |F_{\text{meas}}|$], S [$\sum (\Delta F_{\text{meas}} / \sigma F_{\text{meas}})^2 / (m-n)^{1/2}$], † and other indicators.
 - (d) Treatment of unobserved reflexions; worst agreement between F_{calc} and unobserved reflexions.

IV. Structural results

1. Atomic coordinates; ratio of largest shift in last refinement cycle to standard deviation in coordinate given.
2. Thermal parameters (explicitly defined) and occupancy factors (if varied).
3. Interatomic distances, angles and other molecular-geometry features of major interest, including intermolecular distances; if corrections for thermal motion are made also give uncorrected values.
4. Diffraction data indicating disorder and other evidence of disorder.

V. *Structure factor tables.* Crystal-structure papers are incomplete without the evidence contained in the F_{meas} . These tables should include at least hkl (in some form), $|F_{\text{meas}}|$, and preferably but optionally $|F_{\text{calc}}|$. Photographic direct reproduction permits at least 2000 legible full structure factor entries per journal page.

$$* \Delta F_{\text{meas}} = ||F_{\text{meas}}| - |F_{\text{calc}}||.$$

† m = number of ΔF_{meas} , n = number of variables.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

The Jahn–Teller effect in molecules and crystals. By R. ENGLMAN. Pp xvi+350 London: Wiley, 1972. Price £8.00.

The Jahn–Teller effect has received a great deal of attention and new understanding in the last few years. The recent progress has been made largely by new insight into the workings of the effect and the way it modifies the physical properties of systems to which it applies, namely those with degenerate or nearly-degenerate electronic states, rather than by any new mathematical formulation of the theorem itself. Much of this progress has revolved around the dynamic nature of the ‘vibronic’ coupling between electronic and vibrational motions, and with the introduction of new concepts the theoretical aspects of the problem have become quite complex.

This book, by a theoretician who has made a number of important contributions to several aspects of the subject, has as its objective ‘to present all or most aspects of the modern Jahn–Teller effect’. This is a worthwhile aim, since most other reviews of the subject concentrate on applications to a limited class of systems, e.g. defects in solids, molecules, or extended systems. The author feels that there

is bound to be an advantage in collecting together in one volume examples of the Jahn–Teller effect in different systems, and it is certainly interesting to be able to compare the view of the Jahn–Teller effect as seen from different vantage points. Although a variety of physical systems are included, the intention is to concentrate on the way in which the Jahn–Teller effect operates, rather than to describe in detail the physics of each system.

The degree of success in meeting these objectives varies throughout the book. In no way is this a text for the beginner attempting to get a ‘feel’ for the Jahn–Teller effect and an introduction to the theory. The approach throughout is to rely on references to the original work for details, and to some extent the mathematical formulation is influenced by a degree of hindsight and familiarity with the techniques involved. This is especially true in the two short introductory chapters and the long chapter 3, which presents the mathematical solutions to Jahn–Teller and pseudo-Jahn–Teller problems in localized systems (i.e. molecules and defects in solids). The jumping-off point for the theory is fairly advanced, and a slightly annoying feature of chapter 3 is the need to refer constantly to chapter 7 for details of the physical systems used as examples. This same problem

also occurs in the later chapters. To be fair the author makes apology for the rather arbitrary placing of chapter 7 (called *The Physical Landscape*), but this is little comfort to the reader who constantly has to flick forward a hundred pages or so for details of systems with which he is unfamiliar. Personally, I would have preferred the chapter to have preceded chapter 3, so that the basic features of the systems are described before getting involved with their Jahn–Teller properties.

Chapter 4 is a mixed bag of examples of the behaviour of Jahn–Teller systems under stress, including the (often crucially important) effect of internal random strains in crystals. Chapter 5 presents a very useful account of the operation of the Jahn–Teller effect in extended systems, examining the relation between vibronic coupling and symmetry-lowering crystallographic phase transitions. This is a difficult branch of the subject, since it would seem that few distortive effects in extended systems have a unique interpretation. Nevertheless the author manages to present a critical review which should equip the reader for a more detailed pursuit of these topics. Chapter 6 discusses relaxation problems. Again the treatment is probably rather abbreviated for the uninitiated, relying heavily on the references. The book ends with nine appendices, including a collection of data on Jahn–Teller systems, which forms a valuable feature of the book as a reference text.

Despite the rather uneven success rate at getting the material across to the reader, this book will be a useful text for research workers involved directly or indirectly with the various manifestations of the Jahn–Teller effect. The references are comprehensive and there are many instances where recent, sometimes unpublished, work is included. Dr Englman has made a significant step forward in preparing a book of this type, and its few shortcomings are mitigated by its unique place in the Jahn–Teller literature.

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Optical transforms. Edited by H. S. LIPSON. Pp. xi + 436, London: Academic Press, 1972. Price £7.25.

It is a quarter of a century since work began in Manchester on the application of optical transforms to X-ray crystallography under the guidance of Professor Lipson. At that time the effort was concentrated on the solution of crystal structures by matching optical transforms to weighted reciprocal-lattice sections and some work was also done in producing optical Fourier syntheses. The advent of the computer and the development of better techniques for solving crystal structures rendered this activity out of date by the mid 1950's. However that was not the end of optical-transform research: since that time it has been applied to an ever wider variety of problems and this book is devoted to a description of what can be done, and what can be better understood, by working or thinking in terms of optical transforms.

The book consists of a series of articles, written by ac-

knowledgeable experts in their fields, and many of them protégés of Professor Lipson. Each article deals with a particular topic and they are so written that they are complete in themselves and can be read without reference to each other.

The titles of the chapters and their authors are as follows:

1. *Basic principles* by H. Lipson.
2. *Coherence requirements* by B. J. Thompson.
3. *Determination of crystal structure* by B. Chaudhuri.
4. *Polymer and fibre diffraction* by C. A. Taylor.
5. *Biological studies* by J. A. Lake.
6. *Optical Fourier synthesis* by G. Harburn.
7. *Low energy electron diffraction* by W. P. Ellis.
8. *Optical data processing* by B. J. Thompson.
9. *Holography* by J. Shamir.
10. *Optical transforms in teaching* by S. G. Lipson.
11. *Miscellaneous applications* by J. E. Berger, C. A. Taylor, D. Shechtman and H. Lipson.

The overall quality of the writing is very high and the illustrations are excellent and numerous – a credit to the authors and to the publisher. In the view of the reviewer Chapters 3 and 6 can be regarded only as of historical interest and should have had less space and detail devoted to them.

Covering such a wide field there is something for nearly everybody in this work and it can be wholeheartedly recommended to those interested in any aspect of optics or diffraction.

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LEED – Surface structures of solids, Parts 1 & 2.

Edited by M. LAZNIČKA. Part 1: Pp.431; Part 2: Pp. 470. Prague: Czechoslovak Academy of Sciences, 1971. Obtainable from JČMF, Spálená 26, Praha 2, Czechoslovakia. Price approximately \$16.

At the beginning of September 1971 the Czechoslovak Academy of Sciences held a Summer School on Low Energy Electron Diffraction in Smolnice, Czechoslovakia. They chose to do so because it was their opinion that LEED had reached a stage in its development when a summarizing point of view could be practically and usefully attempted. To undertake this task they invited as speakers and teachers those physicists who have played a prominent role in the theoretical and experimental work completed on LEED since the mid 1960's when the present upsurge in interest in LEED started. These two volumes represent the proceedings of the formally taught part of the school and the quality and timeliness of the material they contain reflect great credit on the judgement of the school's organizers. The proceedings contain material with a strong emphasis upon helping the reader to understand, rather than be blinded by, the difficult material of LEED theory. As appears to be unavoidable in Summer schools with an international set of teachers who cannot give a great deal of time to coordination between themselves, the standard of different contributions varies rather widely and the experimentalists come off