geometries to considerations of non-valence forces and related matters such as lattice dynamics and transport phenomena. Notwithstanding the very recent renaissance of accurate experimental and theoretical electron density analyses of organic and inorganic molecules, this trend was inevitable since the basic quantum chemistry necessary for the interpretation of intramolecular bond lengths is well understood whereas non-valence forces have yet to yield to anything like a comprehensive treatment. Kitaigorodskii in his *Organic Chemical Crystallography* must be given enormous credit for anticipating this movement: with very simple geometrical models, he persuaded us that organic crystal structures could often be rationalized and predicted and that the field was ripe for quantitative development.

This new book, which many must have been looking forward to reading, is, by the author's admission, a 'somewhat one-sided' account having 'some degree of imbalance' based, as it is, almost entirely on the atom–atom approach to quantitative calculations of non-valence interactions. The subject is introduced *via* a summary of crystal structures. We see here the difference in emphasis between the workers of Kitaigorodskii's school and (perhaps) mainstream ideas. Organometallic crystals are thought to be built up from molecules with 'anomalous atom-group of atoms' bonds although the architectural principles are obviously those of simple organic crystals. It is suggested that hydrogen-bond energies should be estimated through a comparison of observed and calculated (pair interaction) lattice energies, although the rationale for extending atom–atom calculations to hydrogen-bonded materials has not been established in detail. There are implications that there is considerable ground-state charge transfer in molecular complexes such as anthracene–trinitrobenzene but no clear evidence on this point is available.

Lattice energies are dealt with in Chapter 2. Dispersion, repulsive and multipolar interactions are summarized clearly but it seems a pity that more illustrative attention was not paid to the pretty rigorous calculations available for crystals of the rare gases and simple diatomics. Kitaigorodskii is on much happier ground when he turns to the lattice energies of aromatic hydrocarbons and the summary of the structures of benzene, naphthalene and anthracene is very good. The sections dealing with lattice dynamics and thermodynamics are the best in the book, summarizing very nicely many of the interesting approaches of the past few years and, given the advent of inelastic neutron scattering and other novel spectroscopic methods, pointing the way for future developments.

The discussion of structural methods is, by contrast, misplaced and outdated with the 'spin-off' of the article of fifteen or so years ago on 'Is super-refinement legitimate?' showing through; it is unreasonable surely to discuss, for example, the sphericity of atoms without a careful discussion of the recent combination of neutron and X-ray methods to determine valence electron distribution and effectively to bracket Dawson's unequivocal analysis of the situation in the diamond with the much less accurate structure determination of anthracene.

The conformations of organic molecules and of peptides and proteins are discussed finally. What is perhaps the most useful quantitative approach to the conformational analysis of simple hydrocarbons *viz.* the Lifson consistent force field scheme, is sketched all too briefly and we see little evidence of the more confident predictions of semi-empirical molecular orbital theory. It would have been valuable also to emphasize the entropic contribution to biomacromolecular structure rather than continue to press for *a priori* analyses based on minimum enthalpy criteria.

A reviewer is almost required to be carping. That this is a useful book goes without saying but its seminal influence will depend upon whether Kitaigorodskii is right again and that one's reservations about the atom–atom approach are revealed, retrospectively, to be myopic prejudices.

R. MASON

School of Molecular Sciences
University of Sussex
Falmer
Brighton BN1 90 J
England

Molecular structure by diffraction methods. Vol. 1.

By G. A. SIM and L. E. SUTTON (Senior Reporters). Pp. xvi + 824, Figs. 174, Tables 71. London: The Chemical Society, 1973. Price £15·00.

The Chemical Society has a long tradition of assisting in the task of keeping up with the scientific literature by publishing its *Annual Reports on the Progress of Chemistry*. These had grown so large by 1967 that it was decided in that year to restrict *Annual Reports* to a critical discussion of the significant advances in the major areas of chemistry and to issue in addition a series of *Specialist Periodical Reports* to provide comprehensive cover of the literature for the specialist research worker. These reports will appear annually or, in some cases, biennially for each subject. The present volume is the first in the series on *Molecular Structure by Diffraction Methods* and it basically covers the literature published from January 1971 to March 1972.

It is divided into three parts: *Electron Diffraction*, *Neutron Diffraction* and *X-ray Diffraction* and since the annual output of papers relevant to the first two parts is relatively small their coverage has been extended to include also detailed reviews of earlier work (back to about 1965 in the case of electron diffraction). This is appropriate because structural results by electron and neutron diffraction have not been systematically reviewed since the publication of the supplementary volume of *Tables of Interatomic Distances and Configuration in Molecules and Ions* which covered the literature up to the end of 1959. The part devoted to electron diffraction has chapters discussing theory and accuracy and the interplay between spectroscopy and electron diffraction as well as two chapters describing structural results. In all, 686 references are discussed in this part, including 464 devoted to results. The two striking features of this part of the report are the complexity of the molecules which can now be studied by electron diffraction and the accuracy of the dimensions which can be obtained.

The short but lively part devoted to neutron diffraction discusses 96 references. As might be expected, most of these are concerned with the accurate determination of hydrogen-atom positions and they are discussed mainly under two headings: *Conformation and Other Stereochemical Problems* and *Hydrogen-Bonded Systems*. Among the other sections is a very interesting one on the application of neutron diffraction in the study of molecular electron-density distributions.

The third, and by far the largest, part is devoted to structural results of X-ray diffraction. In this part, two contributors discuss organic structures (631 references), two describe the structures of globular proteins (a surprisingly large total of 40 high-resolution structures and 146 references) and four contributors deal with inorganic structures (1228 references). Many of the structures are illustrated, a few by stereoscopic views, and there are many informative tabulations of dimensions of related structures. In the sections on inorganic compounds one chapter is devoted to each group in the periodic table but the chapter which includes silicon does not discuss silicate structures containing infinite networks of SiO_4 tetrahedra. There is also a chapter on mixed-cluster complexes.

Although the price is rather high it is reasonable when one considers the wealth of information that the volume contains and the tremendous effort which must have been put into compiling it. The time can be foreseen when this effort will become unnecessary, when the publication of numerical data for organic and organometallic structures by the Crystallographic Data Centre at Cambridge in the series *Molecular Structures and Dimensions* comes up to date and when there is also a comparable publication for inorganic structures. Meanwhile, the volumes in the present series will serve a very useful purpose in surveying briefly the whole structural field and in bringing together information about related compounds. Perhaps the best commendation is that, in spite of attempting to skip through the book rapidly, the reviewer continually found himself attracted to reading paragraphs or larger sections in detail.

S. C. WALLWORK

Department of Chemistry
The University
Nottingham NG7 2RD
England

Molecular structure and dimensions. Edited by OLGA KENNARD and DAVID G. WATSON. Utrecht: Oosthoek, 1970. Vol. 1: pp. xxiii + 489; price £6·50, (personal) £4·50. Vol. 2: pp. xxiii + 344; price £5·00, (personal) £3·75. Vol. 3: pp. xxiii + 490; price £7·75, (personal) £5·50. Vol. 4: pp. xiii + 465; price £7·75, (personal) £5·50.

Among the different areas covered by crystallography, crystal structure analysis is certainly one of the most important not only for crystallographers but also for researchers working in other fields of science such as chemistry, physics and biology. This is because diffraction methods are the only ones which give a direct picture of molecular structures. The enormous increase in the number of crystal structure analyses, particularly now that automation of data collecting, of computing and of application of direct methods is available, makes it important that structural information should be systematically collected, classified and made available to all scientists interested in molecular structures. The work of the Crystallographic Data Centre at Cambridge in this respect is certainly of outstanding importance by virtue of both the organization and the comprehensiveness of information. It can be summarized under the following classifications: (i) classified bibliography, (ii) interatomic distances (bond lengths, bond angles, torsion angles, stereo diagrams, *etc.*), (iii) structural numerical data (unit-cell data, atomic coordinates, bond lengths, *etc.*), (iv) computer services (bibliographic file, numerical data file), in which the organic and organometallic (including metal complexes) crystal structures, published from 1960 onwards, are considered.

The four volumes dealing with bibliography are therefore only part of the whole system and their function is better understood in conjunction with the other parts, particularly with the numerical tables, the first volume of which (Vol. A1, *Interatomic Distances* 1960–1965, *Organic and Organometallic Crystal Structures*: this volume gives data for about 1300 structures) has recently been published.

The first two volumes of the bibliographic series, covering the period 1935–1969, have already been reviewed by C. K. Prout [*Acta Cryst.* (1972). B**28**, 2305] and his comments on them are supported by the present reviewer. Volumes 3 and 4 deal with crystal structures published in the periods 1969–1971 and 1971–1972 respectively, but a number of structures published prior to 1969 and omitted from the previous volumes are also included. Entries are arranged in 86 chemical classes and there are three cumulative indexes in each volume: formula, transition-metal and author indexes, which also include the references to entries given in the previous volumes. The classification, even if sometimes questionable, being frequently a matter of personal opinion, is particularly useful not only for retrieving the particular works the reader is interested in, but also to give a general view of what has been of recent interest in structural research in many fields of chemistry. Not only crystallographers, but also organic and complex chemists must feel deeply indebted to the Crystallographic Data Centre at Cambridge for this work.

M. NARDELLI

Istituto di Chimica Generale ed Inorganica
Università degli Studi di Parma
Via M. D'Azeglio 85
43100 *Parma*
Italy

Кристаллография и кристаллохимия. Выпуск 2. Ученые записки Ленинградского Университета № 377. (Серия геологических наук, выпуск 14.) [Crystallography and crystal chemistry. Part 2. Scientific papers of Leningrad State University No. 377. (Geological science series, part 14.)] Pp. 156, Figs. 66, Tables 22. Leningrad Univ. Press, 1973. Price not given.

The requirement that candidates for research degrees should have published papers has led to the proliferation of periodicals issued by Soviet universities for that purpose. The present book contains two dozen papers, chiefly on growth phenomena in inorganic salts, by V. A. Frank-Kamenetskii, his colleagues and students at the Department of Crystallography of the Geological Faculty of Leningrad