

Table 2. *Rotation pattern data for L-isoleucine*
(Zero layer line and first layer line)

Line number	Intensity	d_{obs}	d_{calc}	hkl
1	<i>s</i>	14.15 Å	13.89 Å	100
2	<i>s</i>	6.972	6.945	200
3	<i>vs</i>	4.849	4.832	230
4	<i>vw</i>	4.695	4.746	140; 300
5	<i>vs</i>	4.467	4.503	310
6	<i>vw</i>	4.191	4.173	320
7	<i>vw</i>	4.040	4.031	050
8	<i>vs</i>	3.842	3.875	150
9	<i>vs</i>	3.506	3.489	250
10	<i>w</i>	3.251	3.268	160
11	<i>vw</i>	3.099	3.083	430
12	<i>vs</i>	2.812	2.832	170
13	<i>w</i>	2.714	2.721	360
14	<i>m</i>	2.528	2.522	080
15	<i>w</i>	2.426	2.421	540
16	<i>s</i>	2.364	2.369	280
17	<i>vw</i>	2.241	2.242	090
18	<i>vw</i>	2.103	2.106	640
19	<i>vw</i>	2.004	2.008	650; 570
20	<i>vs</i>	4.794	4.854	111
21	<i>m</i>	4.674	4.733	021
22	<i>s</i>	4.517	4.480	211
23	<i>vw</i>	4.052	4.013	131
24	<i>s</i>	3.918	3.911	221
25	<i>s</i>	3.657	3.673	041
26	<i>w</i>	3.314	3.272	321
27	<i>vw</i>	3.217	3.224	051
28	<i>uw</i>	3.088	3.107	331
29	<i>vs</i>	2.860	2.848	061
30	<i>s</i>	2.793	2.800	421
31	<i>vw</i>	2.625	2.635	261
32	<i>vw</i>	2.492	2.499	171
33	<i>w</i>	2.421	2.425	361

reliability of an indexed powder pattern gave $M_{20}=7.6$, where $(10^4 \sin^2 \theta)_{20}=934$, $X_{20}=0$, $N_{20}=28$, and the discrepancy in the $10^4 \sin^2 \theta$ value, $\bar{\epsilon}=2.20$. The number of observed lines below $(10^4 \sin^2 \theta)_{20}$ is 26% of the theoretically expected number and the actual discrepancy in this range is 0.28 times the average expected discrepancy calculated by de Wolff's (1961) method. This corresponds to a probability of 10^{-12} for an alternative lattice of the same size. The cell data derived are thus substantially correct. No systematic absences among observed reflexions could be found except $00l$ for $l=2n+1$. The probable space group is $P22_1$.

The crystal structure of D-leucine (Möller, 1949) is based on double-layer units stacked along the b axis, where $a=5.36$, $b=14.70$, $c=9.65$ Å; space group $P2_122$ or $P22_2$, and $Z=4$. Comparing present data, the molecules of L-isoleucine are expected to pack in double-layer units parallel to the bc plane, with the length of the chain along the a axis, as proposed for DL-isoleucine (Dawson & Mathieson, 1951).

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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.

Infra-red spectra and structure of organic long chain polymers. By ARTHUR ELLIOT. Pp. viii + 119. London: Arnold, 1969. Price 35 s.

This book deals exclusively with one topic – the infrared-spectroscopic study of polymer structures of organic and biological origin.

The author considers in some detail the practical aspects of obtaining polymer spectra – choice of spectrometer, utilization of polarized radiation, preparation of samples, methods of drying and deuterioexchange, etc. Special attention is given to the question of dichroism in the infrared-spectra of polymers, polypeptides and some proteins (*i.e.* to the field in which the author of the book has acquired a worldwide reputation.)

Special aspects of polymer spectroscopy are treated separately – hydrogen-bond formation, vibrational modes in the amide (peptide) group and the variation of the frequency of infrared absorption with the conformation of polypeptides and polyamides.

Theoretical methods of polymer infrared-spectra analysis are presented very briefly – the symmetry of chain vibrations selection rules, intensity and polarization of vibrations.

The book is written in perspicuous language and is well illustrated; the bibliography includes 143 references. It will be found useful by experts in infrared spectroscopy as well as by anyone investigating the physico-chemical properties and structure of polymers and biopolymers.

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Methods of molecular quantum mechanics. By R. MCWEENY and B. T. SUTCLIFFE. Pp. ix + 307. London: Academic Press, 1969. Price 84 s. \$ 13.50.

This book is the second volume in a series of monographs on theoretical chemistry with consulting editors D. P. Craig and R. McWeeny. The book contains 9 chapters: Introductory survey, Mathematical methods, Many-electron wave functions, Digression: the nature of the electron

distribution, Molecular orbitals and the self-consistent field, Valence bond theory, Some recent developments, Electric and magnetic effects, The calculation of electronic wave functions, and 4 appendices: Quantum mechanical principles, Atomic orbitals and angular momentum, Symmetry and group concepts, Relativistic terms in the Hamiltonian. At the end of the book there are author and subject indexes.

There are many books on the market on these subjects. The great value of this book, however, lies in the way of presentation which is pedagogical and clear. The task of covering the large number of subjects in a relatively short book has been achieved by placing the emphasis on explanation and interpretation rather than detailed derivation. This is particularly evident in the first four chapters and in the appendices. Simple and illustrative examples are worked through; however, exercises especially set for the reader would have improved the book. The book is intended to be self contained and this is fulfilled if the reader has a good background in elementary quantum mechanics or is prepared to take a rather large number of statements for granted. After each chapter there is a reference list to the key literature so the reader has some guidance in finding more detailed treatments.

The subject index at the end of the book is somewhat incomplete and the reader may look in vain for subjects which are in fact treated in the book.

For the crystallographer who is intending to look for details in the electron distribution the book should be a very good introduction. It gives a unified and clear survey of the methods available for calculating electron distributions and of the limitations of these methods.

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Structure and bonding. Volume 6. Edited by P. HEMMERICH, C. K. JØRGENSEN, J. B. NEILANDS, R. S. NYHOLM, D. REINEN & R. J. P. WILLIAMS. Pp. 159. Berlin: Springer-Verlag, 1969. Price (soft cover) DM 34, \$ 8.50.

This volume contains the following papers: *Valence-Shell Expansion Studied by Radio-Frequency Spectroscopy* by E. A. C. Lucken; *Ligand-Field Spectroscopy and Chemical Bonding in Cr³⁺-containing Oxidic Solids* by D. Reinen; *Spectra of 3d Five-coordinate Complexes* by M. Ciampolini; *Valence-Shell Expansion Studied by Ultraviolet Spectroscopy* by C. K. Jørgensen; *Polynuclear Complexes of Iron and their Biological Implications* by Th. G. Spiro & P. Saltman and *Ionic Radii and Enthalpies of Hydration of Ions* by D. F. C. Morris.

Drs Lucken and Jørgensen present very carefully considered reviews of experimental and theoretical data relating to the extent of $p_{\pi}-d_{\pi}$ and $p_{\sigma}-d_{\sigma}$ contributions to bonding. After reading these papers the reviewer found himself in agreement with Dr Lucken's conclusive remark: '... in very few of the examples presented it has been possible to provide *clear* (my italics) evidence for outer d -orbital participation in bonding...'

A very thorough discussion of the electronic spectra of chromium (III)-containing solids is given by Dr Reinen who

shows that a satisfactory interpretation of spectral parameters in compounds of this type must go beyond a ligand-field approach and, perhaps, even beyond a simple molecular orbital approach.

The spectra of 3d five-coordinate complexes receives a lucid and comprehensive treatment by Dr Ciampolini and Drs Spiro and Saltman present an account of the interesting and difficult field of polynuclear iron complexes. Their discussion of the biological implications is tantalizing as it shows how little we know about such 'vital' compounds.

The volume closes with a 'mini-contribution' by Dr Morris, which is an appendix to his earlier review on the same topic in Volume 4 of this series, and serves to set the record straight about the neglect of an earlier contribution by K. Fajans. All in all, this volume makes very interesting reading.

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Solid phase peptide synthesis. By J. M. STEWART and J. D. YOUNG. Pp. xi + 103. Kent, England: Freeman, 1969. Price 48 s.

The book comprises three chapters. The first deals with basic principles of solid phase peptide synthesis, the choice of protecting groups and methods of coupling. The second and third give a detailed account of laboratory techniques and apparatus used in solid phase synthesis. There are also useful appendices dealing with addresses of suppliers of glassware, apparatus, chemicals and reagents, the molecular weights of amino-acids and derivatives, formulae of protecting groups and reagents, and a list of representative peptides prepared by the method. The presentation is crisp and clear, and the inexperienced reader must be left with the impression that peptide synthesis is now delightfully straightforward. Indeed, now that commercial automatic synthesizers are available crystallographers may feel urged, with Stewart and Young's instruction manual for guidance, to rush to their benches and prepare that dodecapeptide themselves!

Beware! The scope and limitations of solid phase synthesis are dealt with cursorily in a one-page postscript. In fairness to the authors, information concerning these shortcomings is slow to appear in the literature. Nevertheless there are increasing numbers of people with long experience in the synthesis of peptides who have had a singular lack of success in applying the method to the synthesis of pure peptides of decapeptide size or above. There are also many smaller sequences that present problems.

The reviewer recommends this book only to the crystallographer who is most enthusiastic about his chemistry.

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