Table 2. *Rotation pattern data for* L-*isoleucine*

(Zero layer line and first layer line)

| Line number | Intensity | $d_{obs}$ | $d_{calc}$ | *hkl* |
|---|---|---|---|---|
| 1 | *s* | 14·15 Å | 13·89 Å | 100 |
| 2 | *s* | 6·972 | 6·945 | 200 |
| 3 | *vs* | 4·849 | 4·832 | 230 |
| 4 | *vw* | 4·695 | 4·746 | 140; 300 |
| 5 | *vs* | 4·467 | 4·503 | 310 |
| 6 | *vw* | 4·191 | 4·173 | 320 |
| 7 | *vw* | 4·040 | 4·031 | 050 |
| 8 | *vs* | 3·842 | 3·875 | 150 |
| 9 | *vs* | 3·506 | 3·489 | 250 |
| 10 | *w* | 3·251 | 3·268 | 160 |
| 11 | *vw* | 3·099 | 3·083 | 430 |
| 12 | *vs* | 2·812 | 2·832 | 170 |
| 13 | *w* | 2·714 | 2·721 | 360 |
| 14 | *m* | 2·528 | 2·522 | 080 |
| 15 | *w* | 2·426 | 2·421 | 540 |
| 16 | *s* | 2·364 | 2·369 | 280 |
| 17 | *vw* | 2·241 | 2·242 | 090 |
| 18 | *vw* | 2·103 | 2·106 | 640 |
| 19 | *vw* | 2·004 | 2·008 | 650; 570 |
| 20 | *vs* | 4·794 | 4·854 | 111 |
| 21 | *m* | 4·674 | 4·733 | 021 |
| 22 | *s* | 4·517 | 4·480 | 211 |
| 23 | *vw* | 4·052 | 4·013 | 131 |
| 24 | *s* | 3·918 | 3·911 | 221 |
| 25 | *s* | 3·657 | 3·673 | 041 |
| 26 | *w* | 3·314 | 3·272 | 321 |
| 27 | *vw* | 3·217 | 3·224 | 051 |
| 28 | *vw* | 3·088 | 3·107 | 331 |
| 29 | *vs* | 2·860 | 2·848 | 061 |
| 30 | *s* | 2·793 | 2·800 | 421 |
| 31 | *vw* | 2·625 | 2·635 | 261 |
| 32 | *vw* | 2·492 | 2·499 | 171 |
| 33 | *w* | 2·421 | 2·425 | 361 |

reliability of an indexed powder pattern gave $M_{20}=7{\cdot}6$, 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, $\bar{\varepsilon}=2{\cdot}20$. 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 $P222_1$.

The crystal structure of D-leucine (Möller, 1949) is based on double-layer units stacked along the *b* axis, where $a=5{\cdot}36$, $b=14{\cdot}70$, $c=9{\cdot}65$ Å; space group $P2_122$ or $P222$, 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).

The author is grateful to Dr C Dakshinamurti and Dr M. S. Swaminathan for their interest in this work.

### References


AZÁROFF, L. V. & BUERGER, M. J. (1958). *The Powder Method in X-ray Crystallography*, p. 118–123. New York: McGraw-Hill.

DAWSON, B. & MATHIESON, A. M. (1951). *Acta Cryst.* **4**, 475.

DE WOLFF, P. M. (1961). *Acta Cryst.* **14**, 579.

DE WOLFF, P. M. (1968). *J. Appl. Cryst.* **1**, 108.

LIPSON, H. (1949). *Acta Cryst.* **2**, 43.

MÖLLER, C. K. (1949). *Acta Chem. Scand.* **3**, 1326.

TROMMEL, J. & BIJVOET, J. M. (1954). *Acta Cryst.* **7**, 703.


## 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 deuteroexchange, *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.

G. N. TISHCHENKO

*Institute of Crystallography*
*Academy of Science of the USSR.*
*Leninsky Prospekt* 59
*Moscow B–333*
*USSR*

### 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