

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

Line number	Intensity	$d_{\text{obs}}$	$d_{\text{calc}}$	$hkl$
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>uv</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).

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 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.

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