Fig. 1. Bond lengths.

Table 2. *Bond angles*

N(4)–Ni —N(5)	89·8 (8)°	Ni —N(6)–C(8)	110 (1)°
N(4)–Ni —N(2)	89·0 (8)	Ni —N(6)–C(4)	105 (1)
N(4)–Ni —N(1)	95·4 (8)	Ni —N(2)–C(2)	162 (2)
N(4)–Ni —N(6)	82·9 (7)	N(2)–C(2)–S(2)	171 (2)
N(5)–Ni —N(3)	93·3 (6)	Ni —N(1)–C(1)	169 (2)
N(5)–Ni —N(6)	82·2 (8)	N(1)–C(1)–S(1)	177 (2)
N(5)–Ni —N(1)	87·8 (9)	Ni —N(4)–C(5)	109 (2)
N(2)–Ni —N(3)	86·1 (8)	N(4)–C(5)–C(6)	111 (2)
N(2)–Ni —N(6)	98·6 (8)	C(5)–C(6)–N(6)	108 (2)
N(1)–Ni —N(3)	100·5 (8)	Ni —N(5)–C(7)	107 (2)
N(6)–Ni —N(3)	82·1 (7)	N(5)–C(7)–C(8)	112 (2)
C(6)–N(6)–C(8)	114 (2)	C(7)–C(8)–N(6)	115 (2)
C(6)–N(6)–C(4)	108 (2)	Ni —N(3)–C(3)	112 (1)
C(8)–N(6)–C(4)	117 (2)	N(3)–C(3)–C(4)	108 (2)
Ni —N(6)–C(6)	102 (1)	C(3)–C(4)–N(6)	108 (2)

physically unreal values, and was not continued. Atom coordinates corresponding to the above R index of 0·107 are listed in Table 1, bond lengths are shown in Fig. 1, and bond angles in Table 2.

The standard deviations are still high, but with the one exception of the length C(6)–N(6) all dimensions are now within error of expected values, and the combined data set has given a much more satisfactory picture of the molecule than did either separately.

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An X-ray study of L-isoleucine. By B. KHAWAS, *Division of Agricultural Physics, Indian Agricultural Research Institute,*

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L-Isoleucine crystallized from aqueous solution is orthorhombic, space group $P222_1$. The cell-edge dimensions are $a = 13·89_6$, $b = 20·17_5$, $c = 5·35_9$ Å and the unit-cell contains eight molecules. From a close resemblance of the cell dimensions and space group to those of D-leucine, it is inferred that the molecules of L-isoleucine are stacked in double-layer units parallel to the bc plane with their chain length along the a axis.

The crystal structures of D-leucine (Möller, 1949), DL-leucine (Möller, 1949; Dawson & Mathieson, 1951), and D-isoleucine hydrochloride and hydrobromide (Trommel &

Bijvoet, 1954) have been reported. Dawson & Mathieson, (1951) reported that DL-isoleucine is triclinic. Against the background of the above extensive studies and sufficient

Table 1. *Powder pattern data for* L-*isoleucine*

Line number	Intensity	d	$10^4 \sin^2 \theta$ Observed	Calculated	hkl
1	vs (bd.)	13·81 Å	31	31	100
2	s	6·972	122	123	200
3	m	4·849	253	252	111
				255	230
4	vs	4·695	270	265	021
5	m	4·475	297	292	310
				296	121
6	vw	4·261	327	330	201
7	vw	4·040	364	365	050
				369	131
8	s	3·885	394	389	221
				396	150
9	vw	3·652	446	441	041
10	m	3·548	472	471	141
11	s	3·485	485	488	250
12	vw	3·421	507	507	410
13	m	3·251	562	564	241
14	w	3·138	604	603	151
15	vvw	2·922	696	695	251
				700	401
16	s	2·854	730	726	440
				733	061
17	w (bd.)	2·812	752	746	170
				758	421
18	w	2·687	823	828	002
19	w	2·573	898	901	530
20	vw	2·522	934	933	441
				934	080
21	vw	2·468	976	977	501
22	s	2·375	1054	1058	280
23	vw	2·315	1109	1108	531
				1109	600
24	vw	2·259	1166	1163	322
				1167	620
25	vw	2·185	1245	1240	630
26	vw	2·139	1299	1296	560
27	m	2·103	1344	1342	640; 551
28	m	2·047	1418	1415	471
				1419	381
				1420	191
29	vvw	1·910	1629	1630	362
30	vw	1·877	1687	1685	452
31	vw	1·847	1742	1737	3 10 0
				1743	740
32	vw	1·780	1876	1874	750
33	vvw	1·718	2014	2010	092
34	vvw	1·690	2081	2081	751
35	vvw	1·630	2237	2237	821
36	vvw	1·579	2384	2380	3 12 0
				2388	063
37	vvw	1·525	2556	2553	920

information on the structural parameters of the isoleucine molecule, a preliminary X-ray study of the crystal structure of L-isoleucine was undertaken.

Pure L-isoleucine, obtained from British Drug Houses Ltd. England, crystallizes in thin elongated leaves. An X-ray photograph of these isolated leafy crystals about their longer dimension in an arbitrary position showed few layer line spots. The crystals were therefore fibrous, lacking random orientation about the fibre axis. A powder pattern of these crystals and a rotation diagram about the long axis were taken with Cu $K\alpha$ radiation ($\lambda = 1·5418$ Å).

From a measurement of the layer line separations in the rotation pattern, the fibre repeat distance was calculated to be 5·36 Å. The line positions in the Debye–Scherrer pattern were measured to an accuracy of 0·05 mm, and the observed spacings were accurate up to 0·001 Å near $2\theta = 62°$. The

presence of a higher crystal symmetry (cubic, tetragonal or hexagonal) was excluded by Azároff & Buerger (1958) tests over observed $10^4 \sin^2 \theta$ values (Table 1). Applying Lipson's (1949) method, the following constants were derived, with which all lines in the powder pattern and the arc-like diffraction spots observed (Table 2) in the rotation diagram up to the first layer could be indexed satisfactorily:

$$\sin^2 \theta_{100} = 308·10^{-5},$$
$$\sin^2 \theta_{010} = 146·10^{-5},$$
$$\sin^2 \theta_{001} = 2069·10^{-5}.$$

The cell parameters calculated from the above data are: $a = 13·896$, $b = 20·175$, $c = 5·359$ Å. The measured density is $1·17 \pm 0·05$ g.cm^{-3}, and assuming $Z = 8$ the calculated density is 1·16 g.cm^{-3}. De Wolff's (1968) criterion for the

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	uw	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 $M_{20} = 7·6$, 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, $\bar{\varepsilon} = 2·20$. 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 $a = 5·36$, $b = 14·70$, $c = 9·65$ 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).

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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 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.

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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 w.. e functions, Digression: the nature of the electron