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Crystal Structure of Butyric Acid*

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According to single-crystal three-dimensional X-ray data, *n*-butyric acid crystals at −43 °C. are monoclinic with

$$a = 8{\cdot}01 \pm 0{\cdot}08,\ b = 6{\cdot}82 \pm 0{\cdot}02,\ c = 10{\cdot}14 \pm 0{\cdot}03\ \text{Å};\ \beta = 111^\circ\ 27' \pm 15'.$$

With 4 molecules per unit cell, the calculated density is 1·135 g.cm.$^{-3}$. This structure exists from the melting point down to about −55 °C. where it changes to a second phase of unknown structure. The structure is described in space group $C2/m$. The molecules occur as dimers with the oxygen and carbon atoms in the mirror plane, but with large amplitudes for out-of-plane vibrations. A structure in space group $C2$ is not ruled out by the calculations, but is considered less likely than the structure in $C2/m$. The bond distances, after corrections of up to 0·03 Å for thermal motion, are C–O = 1·22 and 1·35 Å, C–C = 1·54, 1·53 and 1·53 Å (in order from carboxyl to methyl), each ±0·02 Å. The hydrogen bond length is 2·62 Å.

Introduction

The structure of crystals of *n*-butyric acid ($CH_3CH_2CH_2COOH$) has been studied by X-ray diffraction as a sequel to the work on propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962). Butyric acid melts at −5·5 °C. (Timmermans, 1950). Preliminary experiments indicated a phase change in the vicinity of −55 °C. We have not investigated the structure of the low form because the crystal was always twinned or fragmented. This paper reports the structure of the high form, determined at a temperature of −43 °C. Scheuerman & Sass (1960), before learning of our work, obtained similar results for the unit cell and probable space groups.

Experimental procedure

A small quantity of *n*-butyric acid was sealed in a glass capillary 0·3 mm. in diameter and mounted in the same Weissenberg camera that was used in the study of propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962). The melting point of this sample was observed as −7 °C. The discrepancy with the literature value of −5·5 °C. may not be significant, because a very slow rate of cooling gas flow was used at this temperature, and the thermocouple may not have been at the same temperature as the sample.

A single crystal was grown in the usual manner. Rotation and Weissenberg patterns were taken with Cu $K\alpha$ radiation and with rotation about the a axis. The temperature was −43 ± 2 °C. The unit-cell dimensions were determined from a calibrated zero-layer Weissenberg photograph and uncalibrated rotation and higher-layer patterns. The zero-layer photograph was not calibrated directly with a quartz pattern, but with the rotation pattern of the butyric acid sample at −195°. It had been hoped that information could be gathered about the low-temperature form, and it was impossible to preserve the crystal and still make a quartz calibration. The low-temperature zero-layer Weissenberg photograph was in turn calibrated with a zero-layer strip of the rotation pattern of quartz (a = 4·913 Å). The monoclinic angle β was determined by the method of angular lag.

The intensities of various reflections were estimated visually on multiple-film Weissenberg patterns ($h = 0$ to $h = 6$) by comparison with a standard film strip on which the same reflection was exposed for various times. All of these films were 'Ilford Industrial G'. These observations included 353 independent reflections plus 84 others which were recorded as too weak to be observed. No correction for absorption was deemed necessary since μr was estimated as less than 0·15.

The scale factor for each value of h was adjusted as a variable in the isotropic least-squares refinements. Later this scaling was modified as described below to make it consistent with intensities observed on the rotation pattern, which extended only to the third layer.

Unit cell and space group

The monoclinic unit cell dimensions at −43 °C. are:

$$a = 8{\cdot}01 \pm 0{\cdot}08,\ b = 6{\cdot}82 \pm 0{\cdot}02,\ c = 10{\cdot}14 \pm 0{\cdot}03\ \text{Å};\ \beta = 111^\circ\ 27' \pm 15'.$$

Scheuerman & Sass (1960) found the values (at −30 °C.):

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$$a = 8{\cdot}08 \pm 0{\cdot}02,\ b = 6{\cdot}83 \pm 0{\cdot}02,\ c = 10{\cdot}10 \pm 0{\cdot}02\ \text{Å};\quad \beta = 111^\circ\, 9' \pm 12'.$$

The discrepancies are reasonable considering the accuracy which is claimed. With four molecules per unit cell, the density calculated from our data is 1·135 g.cm.$^{-3}$. The density at -12° is reported to be 1·0875 g.cm.$^{-3}$ (Rozental, 1936).

The Laue symmetry, $2/m$, and the systematic absences, *hkl* absent if $h+k$ is odd, correspond to a C-centered monoclinic lattice. The probable space groups are $C2/m$, $C2$, and Cm. A satisfactory refinement was carried out with the assumption of $C2/m$ with each atom (except some of the hydrogen atoms) in the special positions on the mirror plane:

$$4(\mathrm{i}):\ \pm(x, 0, z) + C\ .$$

As described in more detail later, it is difficult to rule out a structure in space group $C2$ with atoms displaced very slightly from $y=0$. However, we report space group $C2/m$ as the most plausible interpretation of the data.

Determination of the structure

A three-dimensional Patterson function showed that the heavy atoms must lie in or near the planes $y=0$ and $y=\frac{1}{2}$. The same conclusion follows from the observation that the intensities, apart from the usual angular dependence and the extinction rule, are not very dependent on k for a given h and l. The assumption of a dimer, like that of propionic acid, situated in the mirror plane of group $C2/m$ led to a trial structure which was consistent with the Patterson function

Table 1. *Structure factors for butyric acid*

In each group of columns are listed l, the observed magnitude of the structure factor, and the structure factor calculated with the anisotropic temperature factors. The scale factors for the various values of h are discussed in the text. The letter 'X' marks a structure factor which was given zero weight in the final calculations. The reflections $20\bar{1}$, $40\bar{2}$, $40\bar{3}$, and $60\bar{3}$ to $6,0,\overline{10}$ were not photographed. Other reflections missing from the lists were too weak to be observed, with limits for detection ranging from 4 to 12 on this scale

H=0

	K=0			K=2			K=4			K=6	
1	390	400	0	677X	905	0	348	306	0	100	82
2	38	35	1	325	278	1	121	107	1	24	32
3	54	-58	2	43	26	3	41	-36	3	17	-16
4	299	-220	3	61	-54	4	73	-73	4	31	-27
5	96	93	4	163	-158	5	16	22			
6	132	109	5	60	64	6	24	29		K=8	
7	21	22	6	83	77	8	16	-13	0	24	20
8	32	-39	7	14	17	9	10	-11			
9	36	-32	8	24	-29						
			9	21	-24						

H=4

	K=0			K=2			K=2			K=4	
-12	10	9	-12	9	7	6	49	48	3	13	-12
-11	7	-9	-10	24	-29	7	14	17	4	16	-10
-10	29	-36	-9	28	-29				5	15	15
-9	36	-36	-8	96	-94		K=4		6	28	26
-8	143	-120	-6	70	77	-10	14	-15	7	7	10
-6	103	102	-5	22	15	-9	14	-16			
-5	12	15	-4	104	111	-8	47	-47		K=6	
-4	180	150	-3	30	-30	-6	35	35	-9	5	-7
-1	126	151	-2	28	-29	-5	15	13	-8	16	-17
0	151	161	-1	102	105	-4	47	53	-6	10	11
1	111	121	0	125	112	-3	12	-11	-5	7	8
3	17	-15	1	75	86	-2	10	-10	-4	20	21
4	22	-22	2	6	0	-1	36	38	-1	9	8
5	40	40	3	17	-15	0	48	40	0	9	6
6	66	60	4	21	-18	1	29	32	1	8	5
7	21	20	5	30	31	2	11	-8	4	7	-3

H=5

	K=1			K=1			K=3			K=5	
-12	8	9	3	38	-40	0	42	45	-1	21	21
-11	9	7	4	31	-32	1	7	-3	0	15	15
-9	10	-2	5	26	-21	2	16	-15	2	7	-7
-8	28	23				3	23	-26	3	12	-13
-7	15	-20		K=3		4	23	-20	4	10	-9
-6	82	81	-11	7	5	5	16	-13	5	5	-5
-5	33	32	-8	10	12						
-3	127	131	-7	18	-17		K=5			K=7	
-2	32	34	-6	39	40	-7	12	-11	-3	12	9
-1	87	83	-5	18	15	-6	12	9	-1	9	7
0	88	81	-3	71	75	-5	7	2			
1	18	-2	-2	18	22	-3	36	30			
2	22	-23	-1	44	50	-2	10	12			

H=6

	K=0			K=2			K=2			K=4	
-12	24	23	-12	21	19	2	40	-43	-1	10	10
-11	18	12	-11	13	10	3	30	-30	0	22	23
-2	19X	33	-8	22	17	4	14	-18	2	22	-20
-1	4	7	-7	32	35	5	8	-6	3	14	-15
0	49	45	-5	6	12				4	8	-10
2	54	-56	-4	87	-79		K=4				
3	41	-39	-3	55	-54	-8	10	8		K=6	
4	19	-22	-2	23	27	-7	16	16	-4	19	-14
5	12	-8	-1	8	9	-4	48	-40	-3	11	-8
			0	34	38	-3	26	-25	0	13	10
			1	7	-6	-2	19	16	2	7	

H=1

	K=1			K=1			K=3			K=5	
-11	13	14	7	22	-19	1	265	265	-3	48	-49
-9	38	36	8	40	-40	2	54	-55	-2	12	-15
-8	41	42	9	42	-35	3	47	-45	-1	12	-11
-7	80	70	10	16	-19	4	99	-94	0	43	43
-6	159	157				5	104	-98	1	88	88
-5	192	155		K=3		7	16	-12	4	34	-32
-4	64	41	-9	26	23	8	18	-23	5	36	-35
-3	204	-212	-8	22	25	9	19	-21	8	8	-8
-2	51	20	-7	35	41	10	8	-11			
-1	196	-133	-6	84	84					K=7	
0	282X	...	-5	76	73		K=5		-3	17	-18
1	471X	581	-4	10	14	-9	8	11	1	21	26
2	187	-148	-3	111	-118	-8	10	10	4	9	-8
3	84	-93	-2	10	-10	-7	15	17	5	11	-10
4	196	-176	-1	23	-40	-6	22	27			
5	211	-177	0	139	131	-5	19	17			

H=2

	K=0			K=0			K=2			K=4	
-11	13	11	8	14	-17	5	13	-14	2	12	-9
-10	20	-12				6	17	-19	3	40	-44
-9	21	-23		K=2		7	10	8	4	26	22
-8	102	99	-10	14	-11	8	17	-15	6	10	-9
-7	69	81	-9	18	-18	9	8	-6	8	12	-9
-6	86	99	-8	77	77						
-5	30	27	-7	54	64		K=4			K=6	
-4	349X	-233	-6	71	78	-9	9	-8	-8	16	14
-3	341	-309	-5	27	19	-8	40	38	-7	15	13
-2	295	-297	-4	173	-164	-7	31	33	-6	13	17
0	304X	-344	-3	171	-213	-6	38	41	-4	16	-19
1	136	-96	-2	247	-210	-5	9	8	-3	18	-23
2	114	-82	-1	48	-55	-4	50	-66	-2	27	-29
3	224	-207	0	225	-213	-3	81	-81	-1	10	-9
4	28	40	1	66	-64	-2	89	-88	0	23	-19
5	21	-22	2	62	-53	-1	26	-23	4	19	12
6	29	-25	3	135	-140	0	84	-71			
7	14	12	4	24	33	1	15	-21			

H=3

	K=1			K=1			K=3			K=5	
-12	12	12	5	140	133	1	57	-41	-2	25	-26
-11	18	-17	6	61	61	2	22	-27	0	16	13
-10	24	-22	7	26	29	3	32	-32	1	25	-19
-9	110	-98				4	19	17	2	14	-13
-8	78	-64		K=3		5	92	81	3	14	-9
-7	96	88	-12	8	8	6	38	38	4	14	9
-6	11	10	-11	13	-11	7	17	17	5	36	33
-5	65	47	-10	18	-16				6	16	16
-4	180	-162	-9	65	-61		K=5		7	8	6
-3	366	-361	-8	37	-37	-10	9	-9			
-2	177	-161	-7	47	55	-9	30	-26		K=7	
-1	8	10	-6	18	16	-8	12	14	-7	8	8
0	106	98	-5	34	37	-7	25	24	-6	7	7
1	80	-72	-4	77	-82	-6	14	14	-5	11	10
2	46	-38	-3	182	-178	-5	20	23	-3	15	-11
3	60	-59	-2	85	-82	-4	26	-23			
4	22	25	0	45	50	-3	50	-54			

and which had coordinates which differed by less than 0·02 from our final values for carbon and oxygen atoms.

The structure was refined by the method of least-squares with the IBM-650 computer using the nearly-diagonal program 'LS-II' (Senko, 1957). Reflections were weighted as in the last cycles of choline chloride (Senko & Templeton, 1960). The atomic scattering factors of Hoerni & Ibers (1954) for carbon and oxygen were used in all calculations. In this program, individual isotropic temperature factors are used.

After many cycles, the conventional unreliability factor R was reduced to 0·167, but the bond distances were unsatisfactory. Addition of hydrogen atoms at assumed positions, with further refinement, reduced R to 0·128. An additional cycle, with hydrogen atoms omitted, gave $R=0{\cdot}159$.

For this structure, C–C bond lengths were 1·48, 1·52, and 1·49 Å, and C–O bond lengths were 1·19 and 1·34 Å. We were dissatisfied with these results.

A three-dimensional difference synthesis showed positive peaks in positions indicating large thermal vibration perpendicular to the mirror plane, or alternatively, small displacements of atoms from this plane. Earlier, attempts had been made to refine the structure in space group $C2$, with atoms slightly displaced from the plane. If the atoms are all nearly in the plane, then each $\partial|F|/\partial y$ is nearly zero, and the program fails to operate properly. If larger displacements are made, the program shifts atoms back toward the mirror plane.

Table 2. *Atomic coordinates and standard deviations*

Atom	x	y	z	$\sigma(x)$	$\sigma(z)$
Oxygen 1	0·2359	0	0·0379	0·0006	0·0004
Oxygen 2	0·9987	0	0·8382	0·0006	0·0004
Carbon 3	0·1582	0	0·8986	0·0010	0·0006
Carbon 4	0·2932	0	0·8248	0·0010	0·0007
Carbon 5	0·2072	0	0·6647	0·0013	0·0008
Carbon 6	0·3471	0	0·5968	0·0012	0·0008

Table 3. *Anisotropic temperature parameters*

Atom	β_{11}	β_{22}	β_{33}	β_{13}
Oxygen 1	0·0334	0·0595	0·0150	0·0061
Oxygen 2	0·0310	0·0470	0·0159	0·0089
Carbon 3	0·0303	0·0298	0·0183	0·0095
Carbon 4	0·0361	0·0466	0·0182	0·0091
Carbon 5	0·0426	0·0651	0·0190	0·0135
Carbon 6	0·0423	0·0501	0·0236	0·0189

At this point in the work, the IBM-704 computer became available to us, and a refinement with anisotropic temperature factors was undertaken with the Busing & Levy (1959) program, using only the observed reflections. Hydrogen atoms were omitted. The scale factors for the layers were taken from the isotropic refinement. After five cycles, shifts were negligible and R was 0·127. The final calculated structure factors are compared with the observed structure factors in Table 1. The final atomic coordinates and temperature parameters are given in Tables 2 and 3.

Discussion of the thermal motion and structure

The anisotropic temperature factor of each atom in the mirror plane is of the form

$$\exp\left(-\beta_{11}h^2-\beta_{22}k^2-\beta_{33}l^2-2\beta_{13}hl\right) .$$

The correct evaluation of the thermal parameters β_{ij} obviously requires proper scaling of the data. By observations from the rotation pattern, it was concluded that the data of Table 1 would be more correct if each observed structure factor were multiplied by the factor $\exp(0{\cdot}0085h^2)$. If this is done, then 0·0085 must be subtracted from each β_{11} in Table 3. Because the layers above the third were not recorded on the rotation photograph, the accuracy of this correction is very poor. The accuracy of the β_{13} values is also doubtful, but the values obtained are plausible. To facilitate the discussion of these parameters, the temperature factors B in the expression $\exp(-B\sin^2\theta/\lambda^2)$ for the principal axes of thermal motion are listed in Table 4. The directions of the principal axes in the ac plane are determined poorly, but for most of the atoms the larger motion in this plane is approximately transverse to the skeleton of the molecule.

Table 4. *Principal temperature factors*

	B		
Atom	(b axis)	(ac plane)	Angle*
Oxygen 1	11·1 Å^2	6·0, 5·0 Å^2	45°
Oxygen 2	8·7	5·9, 4·3	130
Carbon 3	5·5	6·6, 4·2	120
Carbon 4	8·7	6·8, 5·6	140
Carbon 5	12·1	8·1, 5·4	155
Carbon 6	9·3	9·9, 4·1	140

* Angle between c axis and direction of smallest motion, with angle to a axis acute.

In spite of the uncertainty concerning the details of the thermal analysis, it is clear that there is considerable displacement of the atoms from the mirror plane. This displacement is measured by β_{22}, which like β_{33} is relatively independent of the doubtful scale factors. The largest β_{22}, that of atom C_5, corresponds to a root mean square displacement of 0·39 Å. In propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962) the terminal carbon atom is 0·30 Å out of the plane of the rest of the skeleton. We suggest that in the butyric acid crystal the molecules tend to be similarly non-planar, but that the distortions are randomly up and down and that a particular molecule vibrates from one configuration to the other. Even the largest r.m.s. amplitude is not greatly different from the amplitudes of the in-plane vibrations, whose average is about 0·28 Å. This fact makes us consider it unlikely that the molecules could have an ordered structure in space group $C2$ at this temperature. A proper analysis of our suggested structure would require consideration of the effect of the assumed double minimum of the vibration potential on the mathematical form of the temperature factor. To rule out space group $C2$ by the diffraction data (if it could be done) would require further calculation, for example by least squares with consideration of the terms in $\partial^2|F|/\partial y^2$. Circumstances do not permit us to undertake such calculations at this time, and they probably are not justified without more reliable scaling of the data.

This dynamic disorder could not persist at a low temperature. The phase change at −55 °C. goes to another structure which we suggest contains non-planar molecules in a less symmetrical environment.

Table 5. *Bond distances as observed and after correction for thermal motion*

Bond	Observed length	Corrected length
O_1–C_3	1·32 Å	1·35 Å
O_2–C_3	1·20	1·22
C_3–C_4	1·52	1·54
C_4–C_5	1·51	1·53
C_5–C_6	1·52	1·53
O_1–H · · · O_2	2·62	2·62

The large thermal motion tends to make the observed bond lengths shorter than the true values. The correction requires assumptions concerning the details of the thermal motion, but must include a term of the order of $(B_i - B_j)/16\pi^2 d$, where B_i and B_j are the temperature factors for the b-axis direction for the two atoms and d is the bond distance. With the most optimistic assumptions, the in-plane vibrations are unimportant, and the correction ranges from 0·012 to 0·027 Å for the various bonds in the molecule. The observed bond lengths are compared with the corrected values in Table 5. Other kinds of assumptions give larger corrections and unreasonably long bond distances.

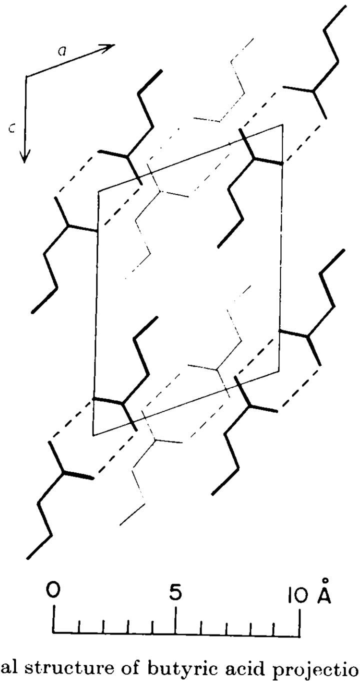

Fig. 1. Crystal structure of butyric acid projection along [010]. The parallelogram indicates one unit cell. The heavy lines represent molecules at $y = 0$; the lighter ones, molecules at $y = \frac{1}{2}$. Broken lines represent hydrogen bonds.

The arrangement of the molecules in the unit cell is shown in Fig. 1, where broken lines represent the hydrogen bonds which connect the molecules of each dimer. The observed molecular dimensions are shown in Fig. 2. Standard deviations are 0·02 Å or less for bond distances and about 1° for bond angles. In these estimates no consideration is given to systematic errors such as the effects of the thermal motion. The inaccuracy of the cell dimensions makes a considerable contribution to these errors.

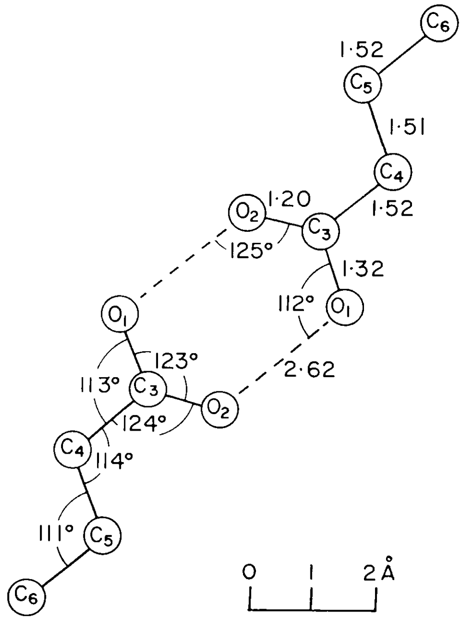

Fig. 2. Observed molecular dimensions, before correction for thermal motion. All atoms shown are in the same mirror plane.

The molecular shape is very analogous to that of propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962). The bond distances were shorter than expected before correction for thermal motion, but are quite normal when corrected.

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The Crystal Structure of Valeric Acid

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A three dimensional X-ray study of crystalline valeric acid has shown it to be monoclinic with

$$a=5\cdot55,\ b=9\cdot664,\ c=11\cdot341\ \text{Å};\ \beta=101^\circ\ 49',;\ Z=4,$$

and space group C_5^{2h}–$P2_1/c$. The trial structure was obtained from a Patterson function of the *a* axis projection. The structure was refined by least-squares methods. The final structure consists of dimers located about a center of symmetry with a hydrogen bond distance of 2·63 Å. The observed interatomic distances are C–O = 1·35, 1·26 Å; C–C = 1·53, 1·53, 1·57, 1·57 Å. All intermolecular contact distances are normal.

Introduction

Recent studies of the crystal structures of formic acid (Holtzberg, Post & Fankuchen, 1953), acetic acid (Jones & Templeton, 1958), propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962) and butyric acid (Strieter & Templeton, 1962) show that the molecular packings of these fatty acids are quite varied. The fact that the melting point of valeric acid ($CH_3CH_2CH_2CH_2COOH$) is lower than that of any other normal fatty acid suggests that either the crystal structure is also of a different nature or that the properties of the liquid state of these acids are largely responsible for their melting behavior. This paper describes the crystal structure of valeric acid as determined by X-ray diffraction. The crystal was found to consist of hydrogen bonded dimers with a molecular packing quite similar to that of propionic acid.

Experimental

Preparation of crystals

Attempts to obtain single crystals of valeric acid using the technique described for propionic acid (Strieter, Templeton, Scheuerman & Sass, 1962) were unsuccessful. However, a much simpler method was devised by which satisfactory single crystals could be obtained in less than an hour's time. Several milliliters of valeric acid were placed in a 30 ml. pear shaped flask. The flask was then placed in a beaker filled with glass beads and the entire assembly set in a Dewar flask filled with crushed dry ice. Under these conditions the valeric acid slowly freezes into well formed crystals. The crystals were broken free from the flask and shaken onto a metal plate cooled by a large block of dry ice. Several small needle-like crystals were selected and placed in 0·3 mm. glass capillaries. A capillary was glued in a brass pin while

Table 1. *Valeric acid atomic parameters*

	Final (isotropic temp. factors)				Final (anisotropic temp. factors)		
Atom	*x*	*y*	*z*	*B*	*x*	*y*	*z*
C_5	0·8162	0·4544	0·1121	5·565	0·8196	0·4553	0·1136
C_4	0·6620	0·3567	0·1817	4·561	0·6607	0·3582	0·1805
C_3	0·5163	0·4428	0·2619	3·678	0·5174	0·4414	0·2628
C_2	0·3857	0·3390	0·3322	3·976	0·3862	0·3400	0·3324
C_1	0·2293	0·4116	0·4066	3·974	0·2208	0·4112	0·4065
O_2	0·1983	0·5405	0·4146	4·593	0·1957	0·5403	0·4146
O_1	0·0971	0·3267	0·4700	4·540	0·0978	0·3280	0·4689