Table 2. *Atomic parameters*

	x/a	*y/b*	*z/c*	B_{11}	B_{22}	B_{33}	B_{12}	B_{23}	B_{13}
C(1)	0·4076	0·0759	0·1294	4·25	3·35	4·00	−0·04	−0·60	0·42
C(2)	0·3553	−0·0183	0·1691	4·79	3·81	5·25	−0·63	−0·23	0·16
C(3)	0·2902	0·0052	0·1110	4·54	5·67	5·95	−1·08	−0·34	−0·07
C(4)	0·2761	0·1213	0·0104	4·60	6·38	5·18	0·08	−0·25	−0·32
C(5)	0·3283	0·2115	−0·0313	5·57	5·29	5·01	0·77	0·07	0·28
C(6)	0·3941	0·1901	0·0251	4·83	4·22	4·78	0·22	0·29	0·49
C(7)	0·5253	0·1367	0·2168	4·48	3·70	4·81	0·00	−0·77	0·36
C(8)	0·5864	0·0770	0·3035	4·95	4·94	6·36	0·17	−0·76	−0·40
N	0·4724	0·0466	0·1981	4·01	3·38	5·12	−0·03	−0·08	−0·04
O	0·5243	0·2580	0·1664	5·61	3·61	7·34	−0·80	0·00	−0·49
H(1)	0·4736	−0·0593	0·2478						
H(2)	0·3660	−0·1097	0·2454						
H(3)	0·2498	−0·0671	0·1438						
H(4)	0·2250	0·1404	−0·0344	Mean isotropic $B=5·04$					
H(5)	0·3176	0·3015	−0·1101						
H(6)	0·4345	0·2611	−0·0114						
H(7)	0·5898	0·1202	0·4285						
H(8)	0·6317	0·1040	0·2340	Mean isotropic $B=8·69$					
H(9)	0·5817	−0·0363	0·3108						

The values of B given above are defined by the expression

$$\exp\left[-\tfrac{1}{4}(h^2a^{*2}B_{11}+2hka^*b^*B_{12}+\ldots)\right]$$

used in the structure amplitude calculations.

Table 3. *Bond lengths and inter-bond angles*

C(1)–C(2)	1·397 Å	C(1)–C(2)–C(3)	120·2°
C(2)–C(3)	1·379	C(2)–C(3)–C(4)	120·4
C(3)–C(4)	1·391	C(3)–C(4)–C(5)	119·0
C(4)–C(5)	1·376	C(4)–C(5)–C(6)	121·7
C(5)–C(6)	1·384	C(5)–C(6)–C(1)	119·1
C(6)–C(1)	1·391	C(6)–C(1)–C(2)	119·6
C(1)–N	1·413	C(2)–C(1)–N	116·6
C(7)–N	1·354	C(6)–C(1)–N	123·8
C(7)–C(8)	1·495	C(1)–N—C(7)	127·6
C(7)–O	1·219	C(8)–C(7)–N	115·3
		N—C(7)–O	123·1
N–H---O′	2·943	C(8)–C(7)–O	121·6
Mean e.s.d. (bonds)	0·0034 Å	Mean e.s.d. (angles)	0·2

This work was made possible by means of a grant from the Department of Scientific and Industrial Research, and we also acknowledge with thanks the help received from Ferranti Limited and International Computers and Tabulators Limited for the gift and servicing of the Pegasus computer.

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On the crystal structures of some α-oxoacids*

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(*Received* 11 *February* 1966)

In continuation of our work on the structures of the sodium salts of α-oxoacids (Tavale, Pant & Biswas, 1961, 1963, 1964), a report on the structural results of sodium salts of (i) 2-oxovaleric acid, $CH_3[CH_2]_2COCOONa$, (ii) 2-oxocaproic acid, $CH_3[CH_2]_3COCOONa$, (iii) 2-oxoheptanoic acid, $CH_3[CH_2]_4COCOONa$ and (iv) 2-oxocapric acid, $CH_3[CH_2]_7COCOONa$ is given.

The crystals of (i), (iii) and (iv) were grown from water–n-butyl alcohol solutions and (ii) from water–isopropyl alcohol solution. They are orthorhombic and grow as very thin plates parallel to the (100) face.

The unit-cell dimensions, space group and number of molecules (n) in the unit cell are given in Table 1, those of the series reported earlier being also given for comparison. Interatomic distances and bond angles of (i) and (iii) are shown in Fig. 1.

Table 1. *Crystal data for the sodium salts of some* 2-*oxoacids*

	a	*b*	*c*	Space group	*n*
Sodium pyruvate	22·25	5·31	3·71	$P2_1/a$	4
Sodium 2-oxobutyrate	29·28	6·05	5·90	*Pbcn*	8
Sodium 2-oxovalerate	34·09	6·14	5·91	*Pbcn*	8
Sodium 2-oxocaproate	39·46	6·11	5·94	*Iba*2	8
Sodium 2-oxoheptanoate	44·18	6·08	5·91	*Pbcn*	8
Sodium 2-oxocaprylate	49·57	6·05	5·97	*Pbcn*	8
Sodium 2-oxocaprate	60·31	6·20	5·96	*Iba*2 or *Ibam*	8

* Communication No. 893 from National Chemical Laboratory, Poona 8, India.

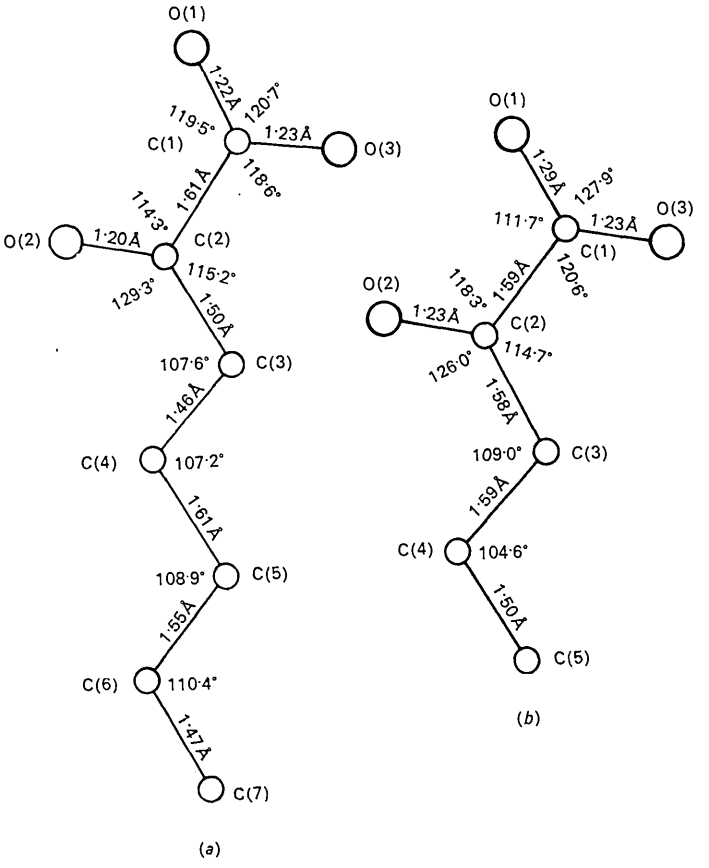

Fig. 1. Bond lengths and bond angles in (*a*) the 2-oxoheptanoate, (*b*) the 2-oxovalerate group. Oxygen atoms O(1) and O(3) are carboxylic and O(2) is ketonic.

Sodium 2-oxovalerate

The observed density at 25 °C measured by flotation is 1·47 g.cm^{-3} and that calculated for eight molecules of $CH_3[CH_2]_2COCOONa$ per unit cell is 1·48 g.cm^{-3}.

Intensity data were collected from zero and higher-layer Weissenberg photographs. The reflexions with $h+k+l$ even are sharp, while those with odd values are diffuse, suggesting the same type of disorder in the crystal as that reported for sodium 2-oxocaprylate (Pant, 1964).

Sodium 2-oxoheptanoate

The observed density at 24 °C, measured by flotation, is 1·37 g.cm^{-3} while the calculated density is 1·39 g.cm^{-3}.

The intensity data indicate that in this crystal also the reflexions with $h+k+l$ even are sharp while those with odd values are diffuse, indicating the same type of disorder as in sodium 2-oxocaprylate.

Sodium 2-oxocaproate and *sodium 2-oxocaprate*

The observed densities at 25 °C for sodium 2-oxocaproate and sodium 2-oxocaprate obtained by flotation are 1·42 and 1·24 g.cm^{-3} respectively while those calculated for eight molecules per unit cell are 1·43 and 1·24 g.cm^{-3} respectively.

The systematic presences for both the substances are: hkl for $h+k+l=2n$, $hk0$ for $h+k=2n$, $h0l$ for $h=2n$, $l=2n$ and $0kl$ for $k=2n$, $l=2n$ suggesting that the space group is either *Iba*2 or *Ibam*.

The reflexions with $k+l=2n$ are sharp while those with $k+l=2n+1$ are diffuse, suggesting thereby that the disorder in these crystals is different from that mentioned earlier.

Structural work on these four compounds is proceeding.

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