structure factors are listed in Table 2. The palladium–chlorine bond length is 2·299 Å, with $\sigma=0{\cdot}004$ Å. This estimate of error allows for uncertainty in both atomic parameter and cell dimension.

Ammonium chloropalladate(IV)

Crystals of $(NH_4)_2PdCl_6$ were obtained, following Sharpe (1953), as small wine-red octahedra. The axial length of the cubic cell was determined from a calibrated rotation photograph as $9{\cdot}84 \pm 0{\cdot}01$ Å, in agreement with Sharpe (1953). The density has been measured as 2·48 g.cm^{-3} (Ketelaar & von Walsem, 1938), and the calculated volume for 4 molecules per cell is 2·476. All crystals comprised several individuals giving rise to multiple spots, and the most suitable that could be found was one for which the separate reflexions coincided over half of the Weissenberg film, at least when the equi-inclination angle was very small. Intensities were measured visually from such spots for the layers *hk*0 and *hk*1. Spherical absorption corrections were applied.

This structure was also confirmed as previously described (Ketelaar & von Walsem, 1938), *i.e.* as in *Fm*3*m* with palladium in (*a*), 0,0,0; nitrogen in (*c*), $\frac{1}{4},\frac{1}{4},\frac{1}{4}$; and chlorine in (*e*), x,0,0, with $x \sim 0{\cdot}23$. Refinement was then as before, except that only the chlorine could adopt anisotropic thermal parameters, and separate scale factors were used for the *hk*0 and *hk*1 data. Eight terms appeared to suffer from extinction and were removed. The *R* index for the 29 terms included was 0·071. The final parameters are listed in Table 1, and observed and calculated structure factors in Table 2.

The palladium–chlorine bond length is 2·300 Å, with $\sigma=0{\cdot}007$ Å.

The assumption that Pd(II) and Pd(IV) have effectively the same atomic radius has thus been confirmed.

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Further refinement of the crystal structure of acetanilide.

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As a result of a number of requests the crystal structure of acetanilide (Brown & Corbridge, 1954) has been further refined. The original X-ray intensity data were used and Cruickshank's (1961) program was used for refining the positional and anisotropic thermal parameters on a Pegasus computer. Seven cycles of structure factors and least squares reduced *R* from 11·2 % to 5·9 % taken over the 1125 observed *F*(*hkl*). The structure amplitude agreement is given in Table 1, the new atomic parameters in Table 2, and the bond lengths and inter-bond angles in Table 3.

The equation of the mean plane through the benzene ring is

$$0{\cdot}2049X - 0{\cdot}5482Y - 0{\cdot}8108Z = 0{\cdot}4229$$

from which the atoms are displaced by C(1) −0·014; C(2) +0·009; C(3) +0·001; C(4) −0·010; C(5) 0; C(6) +0·013 Å. The nitrogen atom is −0·046 Å out of this plane so that the C–N bond makes an angle of 1·9° with the plane of the ring.

The equation of the mean plane containing C(7), C(8), N and O is

$$0{\cdot}3689X - 0{\cdot}2990Y - 0{\cdot}8801Z = 1{\cdot}8978$$

from which the atoms are displaced by C(7) +0·002; C(8) 0; N −0·001; and O −0·001 Å. The normals to these two planes are inclined at 17·6°; the value of 37°54′ given in the previous paper was wrong.

The hydrogen bond, assumed to be linear, makes angles of 110·2° with the N–C(1) bond, 121·9° with N–C(7), and 139·1° with O′–C(7′).

The results of this further refinement seem to indicate an improvement in overall regularity of the molecule; the benzene ring is more nearly regular and more planar; the acetyl group is now planar, and the mean standard deviation of a bond has been reduced from 0·0056 to 0·0034 Å. There is no change in the conformation of the molecule; the mean change in non-hydrogen positional coordinates is only 0·012 Å. This is of interest since in the structure of *N*-methylacetanilide (Pedersen & Pedersen, 1965) the C(8) and O atoms have changed places, together with other differences in molecular geometry. Presumably this *exo* configuration is the more stable one when the oxygen atom does not have to be forced into the *endo* configuration to accept a hydrogen bond.

Table 1. *Observed and calculated structure amplitudes*

H	K	L	F(OBS)	F(CALC)
0	0	2	38.9	-37.4
0	0	4	14.0	15.7
0	0	6	34.3	33.7
0	0	8	2.1	2.0
0	0	10	3.0	3.4
0	2	0	42.5	43.2
0	2	1	97.1	-93.5
0	2	2	77.7	-79.2
0	2	3	14.0	12.4
0	2	4	32.4	-31.8
0	2	5	3.7	-3.8
0	2	6	5.6	-4.8
0	2	7	2.1	-1.9
0	2	10	2.9	2.3
0	4	0	39.9	40.5
0	4	1	44.3	-44.7
0	4	2	9.7	-10.5
0	4	3	2.1	1.3
0	4	4	28.9	-31.5
0	4	5	8.4	8.2
0	4	6	9.9	9.6
0	4	8	5.0	-5.2
0	6	0	19.0	-19.6
0	6	1	4.7	3.9
0	6	2	16.2	17.2
0	6	3	2.4	-1.5
0	6	4	6.9	6.7
0	6	5	5.1	3.8
0	6	6	5.1	-3.7
0	6	9	2.1	1.5
0	8	0	5.3	5.0
0	8	1	3.6	-3.0
0	8	2	5.9	-5.8
0	8	3	4.2	3.9
0	8	4	2.8	-2.4
0	8	5	4.5	-4.9
0	8	7	2.9	-2.4
0	10	0	3.5	-3.3
0	10	1	7.2	8.4
0	10	2	14.2	13.7
0	10	3	5.0	5.1
0	10	5	6.7	-5.9
0	12	0	1.3	1.0
0	12	1	5.6	4.9
1	0	2	84.2	-82.4
1	0	4	18.3	17.2
1	0	6	7.6	6.9
1	0	10	1.3	-1.3
1	1	1	64.8	-64.2
1	1	2	62.6	59.6
1	1	3	33.2	36.1
1	1	4	27.5	-28.4
1	1	5	13.2	-12.5
1	1	6	4.4	4.2
1	1	9	3.1	-2.9
1	1	10	2.2	2.2
1	2	1	80.9	-79.8
1	2	2	82.0	-81.6
1	2	3	29.1	-29.8
1	2	4	11.7	11.8
1	2	5	15.8	-14.5
1	2	6	2.7	2.3
1	2	7	7.8	-6.9
1	2	8	2.1	-1.9
1	2	9	2.8	-2.9
1	3	1	8.9	8.6
1	3	2	7.0	-5.7
1	3	3	37.9	36.3
1	3	4	11.0	9.8
1	3	5	7.7	7.1
1	3	6	1.5	-1.3
1	3	8	4.2	-4.2
1	3	9	2.7	2.9
1	3	10	3.8	3.6
1	4	1	16.6	15.8
1	4	2	15.9	-15.0
1	4	3	23.1	24.6
1	4	4	8.2	8.5
1	4	5	7.6	7.3
1	4	6	6.2	6.0
1	4	7	1.6	1.9
1	4	8	3.3	2.8
1	4	9	2.4	-2.0
1	4	10	1.8	1.7
1	5	1	17.5	-15.2
1	5	2	26.3	23.8
1	5	3	9.5	-9.2
1	5	4	11.9	-11.6
1	5	5	10.9	-10.0
1	5	6	8.1	-7.0
1	5	8	2.9	2.0
1	5	9	1.9	2.2
1	6	1	5.8	-5.2
1	6	2	8.9	-7.0
1	6	3	1.8	-1.8
1	6	4	2.1	-2.3
1	6	7	2.1	2.1
1	6	8	1.5	-1.6
1	7	1	4.2	3.6
1	7	2	7.6	-7.5
1	7	3	12.3	11.9

H	K	L	F(OBS)	F(CALC)
1	7	4	4.5	4.0
1	7	5	7.0	-7.0
1	7	6	7.2	6.1
1	7	7	5.6	4.9
1	8	1	9.5	9.4
1	8	3	2.4	-2.2
1	8	4	3.6	-3.0
1	8	5	3.6	3.7
1	8	6	1.6	1.6
1	9	1	2.2	2.3
1	9	2	4.4	4.3
1	9	3	7.8	-6.6
1	9	4	10.8	-10.4
1	9	5	3.6	2.9
1	9	6	7.2	6.5
1	10	2	4.1	-3.9
1	10	3	8.0	-7.0
1	11	1	2.5	-2.1
1	11	2	7.1	-6.6
1	11	3	3.1	-3.0
1	11	4	3.2	3.6
1	12	2	4.1	-2.8
2	0	0	82.0	81.4
2	0	2	140.3	-142.0
2	0	6	5.2	5.0
2	0	8	9.3	-8.7
2	1	0	51.3	52.4
2	1	1	44.7	45.5
2	1	2	92.8	87.6
2	1	3	30.9	30.3
2	1	4	18.1	16.1
2	1	5	17.9	-17.2
2	1	6	6.3	6.2
2	1	8	5.2	5.2
2	1	9	3.7	3.5
2	2	0	30.5	-29.7
2	2	1	74.5	-69.3
2	2	2	3.9	-4.2
2	2	3	20.8	19.8
2	2	4	26.8	26.0
2	2	5	3.2	-2.5
2	2	6	3.5	-3.3
2	2	7	2.4	-2.0
2	2	8	2.9	-2.4
2	2	9	2.5	1.8
2	3	0	26.2	-26.0
2	3	1	39.9	39.6
2	3	2	4.9	-4.9
2	3	4	26.3	-27.3
2	3	5	9.4	-9.9
2	3	8	5.0	5.3
2	3	9	2.1	-1.5
2	4	0	10.8	11.5
2	4	1	34.5	-34.6
2	4	2	9.5	9.4
2	4	3	10.3	10.4
2	4	4	6.6	5.5
2	4	5	12.7	13.2
2	4	6	14.2	14.2
2	4	9	2.9	2.4
2	5	0	1.5	-1.5
2	5	1	22.2	21.6
2	5	2	1.5	1.7
2	5	3	6.0	-6.3
2	5	4	2.6	-1.9
2	5	5	1.5	-1.4
2	5	6	5.1	-5.7
2	5	7	5.4	4.9
2	5	8	3.2	2.6
2	5	9	1.9	-2.0
2	6	0	36.3	-36.5
2	6	1	2.5	-2.3
2	6	2	11.7	11.7
2	6	3	5.0	-4.2
2	6	4	15.4	15.1
2	6	6	4.5	-4.1
2	6	7	7.1	-6.7
2	7	0	12.8	11.1
2	7	1	2.2	2.2
2	7	3	1.5	-1.6
2	7	4	7.2	7.1
2	7	5	1.5	1.4
2	7	7	2.9	4.1
2	8	0	5.6	-5.4
2	8	1	9.9	-10.2
2	8	2	7.3	-7.4
2	8	3	6.5	7.5
2	8	5	2.1	2.0
2	8	6	3.0	-1.9
2	8	7	2.2	-2.5
2	9	0	16.0	-15.7
2	9	2	3.7	-3.9
2	9	4	3.2	2.8
2	9	5	2.2	-2.6
2	9	6	4.0	-3.4
2	10	0	17.9	-17.2
2	10	2	8.4	7.6
2	10	3	4.1	4.2
2	10	5	2.5	-3.3

H	K	L	F(OBS)	F(CALC)
2	11	2	3.2	3.3
2	11	3	3.6	3.8
2	11	4	5.6	4.5
2	12	1	1.7	1.9
2	12	2	4.2	3.2
3	0	2	40.4	-38.7
3	0	4	13.3	14.0
3	0	6	7.4	-7.8
3	0	8	4.1	-4.1
3	0	10	1.6	-1.4
3	1	1	46.4	48.5
3	1	2	59.4	58.0
3	1	3	11.0	10.7
3	1	4	25.5	-25.9
3	1	5	13.6	-12.9
3	1	6	11.3	11.3
3	1	7	14.1	12.8
3	1	9	2.4	-1.9
3	2	1	16.7	-16.6
3	2	2	32.4	-32.5
3	2	3	34.5	33.8
3	2	4	40.5	40.8
3	2	5	4.5	4.3
3	2	6	2.1	-1.9
3	2	10	1.6	1.5
3	3	1	10.1	-10.2
3	3	2	16.0	-16.4
3	3	3	33.1	-34.6
3	3	4	11.7	-11.9
3	3	5	11.4	-11.0
3	3	6	5.8	5.9
3	3	7	2.1	-2.3
3	3	8	6.3	-6.4
3	4	1	3.2	-3.5
3	4	2	18.9	18.6
3	4	3	33.6	35.9
3	4	4	2.1	2.0
3	4	6	10.1	-10.0
3	4	7	2.1	2.2
3	5	1	27.7	28.5
3	5	2	26.4	26.9
3	5	3	6.9	-7.0
3	5	4	16.3	-14.4
3	5	5	6.0	5.9
3	5	6	4.3	4.5
3	5	8	5.1	4.9
3	6	1	20.3	-20.0
3	6	2	11.5	12.7
3	6	4	4.9	-4.6
3	6	5	11.4	-12.4
3	6	6	5.1	-5.1
3	6	8	3.6	-4.3
3	7	1	3.5	-4.2
3	7	3	6.8	-6.6
3	7	4	2.8	-3.3
3	7	5	3.6	-4.3
3	7	6	2.2	2.4
3	7	7	1.6	1.6
3	8	1	6.5	6.9
3	8	2	17.5	18.7
3	8	3	7.1	-8.0
3	8	4	4.5	-4.3
3	8	6	2.4	2.4
3	9	1	11.2	10.5
3	9	2	11.9	11.9
3	9	3	5.2	-6.4
3	9	4	10.8	-11.2
3	9	5	5.6	4.7
3	9	6	2.9	3.0
3	10	1	10.4	9.4
3	10	3	5.2	-3.4
3	10	5	2.1	2.1
3	11	1	1.8	2.1
3	11	3	4.2	-3.9
4	0	0	26.4	28.2
4	0	2	39.9	-38.1
4	0	4	6.7	5.8
4	0	6	2.1	-1.9
4	0	8	2.1	-1.9
4	0	10	2.7	3.5
4	1	0	68.0	-70.2
4	1	1	32.4	-29.5
4	1	2	6.5	4.5
4	1	4	10.4	-10.8
4	1	6	5.2	-5.6
4	1	9	3.0	2.3
4	2	0	15.1	-15.4
4	2	1	10.8	-10.5
4	2	2	45.2	45.3
4	2	3	22.3	23.4
4	2	4	22.7	24.5
4	2	5	7.8	-7.2
4	2	6	9.2	-9.3
4	2	7	2.9	-2.2
4	2	8	2.1	2.0
4	2	9	2.8	2.8
4	2	10	1.8	1.8
4	3	0	31.1	31.1

H	K	L	F(OBS)	F(CALC)
4	3	1	3.0	-2.4
4	3	2	6.0	-6.3
4	3	3	25.9	-27.1
4	3	4	20.3	-20.8
4	3	5	2.1	1.9
4	3	6	4.7	5.1
4	3	7	2.9	-2.3
4	3	9	2.6	-2.5
4	4	0	3.6	3.1
4	4	1	7.9	-6.3
4	4	2	18.2	-17.7
4	4	3	2.1	2.3
4	4	4	22.2	-21.3
4	4	5	3.7	-3.7
4	4	6	3.7	-3.4
4	4	7	7.1	-7.0
4	5	0	9.2	9.6
4	5	2	7.1	-7.7
4	5	3	10.0	-9.6
4	5	4	3.6	3.1
4	5	5	15.9	15.4
4	5	7	8.1	8.7
4	5	8	1.5	1.4
4	6	0	6.4	-8.2
4	6	4	3.3	-3.4
4	6	5	3.6	4.5
4	6	6	8.1	-8.1
4	6	8	2.6	2.5
4	7	0	23.1	23.5
4	7	1	17.7	-18.1
4	7	2	8.4	-8.0
4	7	3	8.1	-9.0
4	7	4	4.0	4.5
4	7	6	5.6	5.8
4	7	8	1.6	-1.4
4	8	0	25.0	22.7
4	8	1	18.8	-20.2
4	8	2	4.4	5.1
4	8	3	2.6	3.2
4	8	4	3.2	2.2
4	8	5	5.6	5.3
4	8	6	2.9	2.6
4	8	7	2.2	-1.7
4	9	0	6.3	-5.7
4	9	1	6.5	-6.1
4	9	2	1.5	-1.4
4	9	4	2.7	2.7
4	9	5	2.9	2.1
4	10	0	15.9	-14.8
4	10	1	8.9	-9.3
4	10	2	5.4	5.0
4	10	4	2.6	-2.4
4	11	1	3.0	-2.9
4	11	2	3.7	-3.9
4	12	0	3.5	-3.7
4	12	1	2.9	-2.1
4	12	2	2.7	2.7
5	0	4	21.4	-20.5
5	0	6	4.6	-4.8
5	0	10	2.7	-2.5
5	1	1	27.7	-30.3
5	1	2	17.2	16.3
5	1	3	18.3	17.1
5	1	4	38.6	-37.4
5	1	5	17.5	-18.6
5	1	6	2.7	3.8
5	1	7	10.4	10.0
5	1	8	5.7	-5.9
5	1	9	2.8	-2.9
5	1	10	2.5	-2.8
5	2	1	19.4	-20.4
5	2	2	26.4	-25.5
5	2	3	7.0	8.1
5	2	4	19.1	19.1
5	2	5	4.5	-5.1
5	2	7	5.2	-4.1
5	2	8	4.1	4.4
5	3	1	20.5	-19.1
5	3	2	5.7	-5.4
5	3	3	7.8	8.9
5	3	5	6.5	6.0
5	3	6	22.4	22.4
5	3	8	2.4	-1.8
5	4	1	30.0	-27.3
5	4	2	15.2	15.6
5	4	3	11.5	11.6
5	4	4	9.5	-10.4
5	4	5	14.9	-15.1
5	4	6	5.1	-5.1
5	4	7	1.6	1.7
5	4	8	5.8	5.7
5	5	1	2.6	2.7
5	5	2	11.7	11.6
5	5	3	8.6	8.4
5	5	4	12.4	-13.1
5	5	5	19.4	18.9
5	5	6	5.6	5.4
5	5	7	2.1	-2.0
5	6	1	3.6	3.8

H	K	L	F(OBS)	F(CALC)
5	6	2	4.3	4.0
5	6	3	30.4	29.1
5	6	4	5.1	-4.7
5	6	5	4.5	-4.6
5	6	6	4.5	4.1
5	6	7	4.5	5.1
5	7	1	13.8	-12.8
5	7	2	3.1	-3.4
5	7	3	5.8	5.4
5	7	4	2.1	-2.0
5	7	5	5.6	5.9
5	7	6	3.2	-3.5
5	7	7	3.6	-4.0
5	7	8	2.2	-3.1
5	8	1	5.1	-5.2
5	8	2	14.7	13.7
5	8	4	13.8	-12.4
5	8	5	2.6	-2.5
5	8	6	3.2	3.2
5	9	1	5.6	-5.4
5	9	2	11.9	13.0
5	9	3	6.5	-6.4
5	9	5	3.2	3.2
5	10	1	2.8	-2.0
5	10	3	1.9	2.0
5	10	4	2.4	-1.4
5	11	1	2.6	3.4
5	11	3	1.7	1.3
6	0	0	5.8	6.4
6	0	2	37.5	-38.3
6	0	4	6.0	4.9
6	0	6	1.2	1.3
6	0	8	8.2	-8.0
6	1	0	34.1	-35.1
6	1	1	13.9	14.4
6	1	2	18.2	18.1
6	1	3	5.9	7.1
6	1	4	5.8	6.4
6	1	5	1.5	1.7
6	1	6	2.7	-2.6
6	1	7	2.6	-2.4
6	1	9	2.4	-2.4
6	2	0	37.8	-38.0
6	2	1	21.7	19.8
6	2	3	20.9	21.2
6	2	4	9.5	8.9
6	2	5	2.4	-1.7
6	2	6	2.1	-1.9
6	2	7	4.6	4.2
6	2	8	2.7	-2.2
6	2	9	4.7	4.6
6	3	0	55.4	55.5
6	3	1	26.2	27.3
6	3	2	9.7	-8.7
6	3	4	3.7	3.4
6	3	5	9.5	9.6
6	3	6	13.1	12.9
6	3	7	2.9	-2.4
6	3	8	3.1	-3.0
6	4	0	50.1	49.5
6	4	1	14.0	14.6
6	4	2	3.2	3.9
6	4	3	2.8	-3.2
6	4	4	3.7	-4.0
6	4	5	13.0	-13.9
6	4	6	11.2	11.2
6	4	7	7.1	-6.4
6	5	0	12.3	11.8
6	5	1	8.9	8.5
6	5	2	14.9	-14.8
6	5	3	1.5	1.3
6	5	4	8.7	9.0
6	5	5	3.9	-4.5
6	5	6	2.1	-2.3
6	5	7	7.9	-9.0
6	5	8	3.6	-3.8
6	6	0	12.1	12.9
6	6	1	12.3	12.1
6	6	2	8.6	-9.7
6	6	3	4.3	4.8
6	6	4	6.2	-7.0
6	6	7	3.6	3.9
6	7	0	17.1	17.2
6	7	1	9.9	-10.4
6	7	2	19.5	-20.2
6	7	3	14.4	14.7
6	7	4	7.8	-8.3
6	7	7	2.9	-2.8
6	7	8	2.6	-3.0
6	8	0	16.6	17.4
6	8	1	10.6	-11.6
6	8	2	6.9	-7.8
6	8	4	4.3	-4.9
6	8	5	2.1	-1.8
6	8	6	3.2	3.2
6	8	7	1.6	-1.6
6	9	0	2.5	2.6
6	9	1	3.0	-2.3
6	9	2	6.7	6.4
6	9	3	5.8	6.0

H	K	L	F(OBS)	F(CALC)
6	9	6	1.9	1.9
6	10	0	4.7	-6.1
6	10	1	3.7	-3.7
6	10	2	3.7	3.6
6	10	3	1.2	1.2
6	11	0	5.8	6.8
6	11	1	2.1	-1.7
6	11	2	1.4	-1.7
7	0	2	59.4	58.5
7	0	4	3.5	3.3
7	0	6	7.6	8.2
7	0	8	6.7	7.4
7	1	1	16.4	16.0
7	1	2	9.6	9.7
7	1	3	28.2	28.6
7	1	4	18.0	-19.0
7	1	5	20.3	-22.0
7	1	6	3.5	3.4
7	1	7	8.9	8.5
7	1	8	3.3	-3.3
7	1	9	3.9	4.4
7	2	1	30.7	28.7
7	2	2	37.2	-36.6
7	2	4	6.9	7.5
7	2	5	4.3	5.1
7	2	6	14.6	-14.9
7	2	7	2.4	1.7
7	2	8	4.3	-4.2
7	2	9	4.3	4.3
7	3	1	3.3	-2.4
7	3	2	13.5	-13.7
7	3	3	5.2	4.1
7	3	4	3.2	-2.6
7	3	5	13.0	-14.1
7	3	6	9.1	9.7
7	3	7	3.7	-3.1
7	3	8	3.7	-3.9
7	3	9	2.8	3.1
7	4	3	2.5	-3.1
7	4	4	4.5	4.8
7	4	5	10.4	-11.0
7	4	6	2.9	-3.2
7	4	7	4.3	4.7
7	4	8	5.3	6.0
7	5	1	7.6	-6.1
7	5	3	6.0	-6.7
7	5	4	3.5	-3.5
7	5	5	4.5	-5.1
7	5	6	4.0	4.0
7	5	7	4.9	-5.8
7	6	1	8.1	-8.5
7	6	2	17.1	-18.4
7	6	3	8.2	8.0
7	6	4	6.2	7.2
7	6	5	11.1	-11.1
7	6	6	4.9	6.5
7	6	7	4.9	5.1
7	7	1	2.6	2.7
7	7	2	6.5	-7.0
7	7	3	8.5	8.0
7	7	4	5.4	5.3
7	7	7	1.8	-1.3
7	8	3	4.1	4.8
7	8	4	9.4	-9.7
7	8	6	2.6	3.2
7	9	1	2.9	3.4
7	9	6	1.3	-0.9
7	10	1	5.8	-6.0
7	10	3	1.9	2.2
7	10	4	2.9	3.3
7	11	2	3.3	-3.3
7	11	3	1.3	-0.6
8	0	0	23.7	22.8
8	0	2	18.6	-18.3
8	0	4	6.9	6.7
8	0	6	6.7	7.2
8	1	0	59.4	-59.8
8	1	1	20.7	20.7
8	1	2	2.3	4.2
8	1	3	33.7	-35.8
8	1	5	5.2	-5.3
8	1	6	8.0	-8.0
8	1	7	10.6	11.0
8	1	8	3.9	-4.4
8	1	9	6.9	-6.9
8	2	1	1.8	2.1
8	2	2	2.7	3.1
8	2	3	2.7	-2.4
8	2	4	4.1	4.7
8	2	5	6.7	-8.1
8	2	7	2.4	-2.4
8	2	8	2.1	-1.5
8	2	9	1.6	-1.4
8	3	0	8.6	8.6
8	3	1	30.9	30.8
8	3	2	29.3	-30.6
8	3	3	15.2	-16.3

Table 1. (*cont.*)

H	K	L	F(OBS)	F(CALC)
8	3	4	2.1	-1.3
8	3	5	8.4	9.4
8	3	6	3.8	4.6
8	3	7	11.2	12.4
8	3	8	8.0	-9.3
8	4	0	5.4	-4.7
8	4	1	7.1	6.5
8	4	2	12.4	-12.1
8	4	3	3.5	4.0
8	4	4	4.3	-3.8
8	4	5	3.7	3.7
8	4	6	3.3	3.8
8	4	7	4.1	4.8
8	4	8	2.6	-2.3
8	4	9	2.1	1.8
8	5	0	7.8	9.2
8	5	1	7.9	7.3
8	5	2	3.3	-3.7
8	5	3	5.1	-6.2
8	5	4	23.7	24.6
8	5	5	9.2	-9.6
8	5	7	2.1	-2.0
8	5	8	2.3	-3.0
8	6	0	2.9	2.6
8	6	1	5.6	5.5
8	6	3	3.8	-4.1
8	6	4	4.0	4.0
8	6	5	5.5	-5.4
8	6	6	3.0	2.9
8	7	0	13.7	13.7
8	7	1	12.3	-11.4
8	7	2	9.5	-9.3
8	7	3	11.0	11.0
8	7	5	2.5	-2.6
8	8	0	4.0	3.4
8	8	2	4.4	-4.6
8	8	3	2.9	2.6
8	9	0	9.2	-8.8
8	9	1	2.9	-3.1
8	9	2	7.9	8.4
8	9	4	2.1	-2.2
8	9	5	4.0	-4.2
8	10	0	2.9	-3.1
8	10	2	1.4	1.5
8	10	3	1.2	0.5
8	11	1	2.4	-2.3
8	11	3	3.0	-3.1
9	0	2	33.7	35.1
9	0	4	5.8	-6.3
9	0	6	6.5	-5.6
9	0	8	3.1	-2.8
9	1	1	28.1	-28.1
9	1	2	24.0	21.6
9	1	3	5.7	-5.8
9	1	4	13.6	11.0
9	1	5	3.6	3.0
9	1	6	10.6	9.3
9	1	7	5.3	-4.6
9	1	8	6.0	6.1
9	1	9	3.8	-3.9
9	2	1	16.2	18.1
9	2	2	19.3	-18.5
9	2	3	13.6	-13.8
9	2	4	26.9	25.8
9	2	5	5.3	4.2
9	2	6	11.5	-9.6
9	2	8	2.9	-3.6
9	2	9	2.1	2.2
9	3	1	5.2	5.6
9	3	3	10.1	10.5
9	3	4	2.7	-2.2
9	3	5	11.3	11.6
9	3	6	6.3	-7.3
9	3	7	2.4	2.4
9	3	8	1.6	-2.0
9	4	1	5.4	4.4
9	4	2	1.6	-1.0
9	4	3	11.7	-12.9
9	4	4	8.7	9.8
9	4	5	7.1	-7.2
9	4	6	8.0	-8.2
9	4	7	5.8	5.8
9	4	8	2.9	2.7
9	5	1	5.6	4.7
9	5	2	7.1	6.4
9	6	1	2.4	2.0
9	6	2	17.2	-16.9
9	6	3	8.3	8.7
9	7	1	4.3	-5.3
9	7	2	1.7	1.8
9	7	5	3.0	-3.2
9	8	2	3.0	3.8
9	9	1	2.3	1.6
9	10	1	2.9	-2.9
9	10	3	2.4	2.3
9	11	1	3.0	-3.3
10	0	0	34.8	33.9
10	0	2	15.1	15.7
10	0	4	5.3	-5.7
10	0	6	2.9	-2.3
10	0	8	5.5	5.3
10	1	0	35.9	-34.8
10	1	1	30.2	30.3
10	1	2	14.6	15.6
10	1	4	5.8	6.6
10	1	7	7.9	7.2
10	1	9	2.1	-2.0
10	2	1	18.9	-18.5
10	2	3	7.6	-7.8
10	2	4	9.7	-10.1
10	2	5	2.1	2.2
10	2	6	7.4	-6.7
10	2	7	2.4	-1.4
10	2	8	4.1	3.9
10	2	9	1.6	-2.0
10	3	0	43.2	44.9
10	3	1	24.6	26.0
10	3	3	13.6	-13.6
10	3	4	6.3	5.2
10	3	5	4.4	-4.9
10	3	6	9.6	10.6
10	3	7	2.7	-3.1
10	3	8	3.3	-3.7
10	4	0	9.3	-9.3
10	4	1	15.3	-15.2
10	4	2	4.3	4.5
10	4	5	11.0	10.7
10	4	6	6.3	-5.8
10	4	7	4.0	3.1
10	5	1	12.5	11.5
10	5	2	18.0	-18.2
10	5	3	5.8	6.1
10	6	0	5.6	-5.8
10	6	1	5.6	-4.9
10	6	2	12.2	11.4
10	6	3	3.8	-4.1
10	7	0	15.8	14.4
10	7	1	12.5	-11.8
10	7	2	9.5	-10.4
10	7	3	7.4	8.6
10	8	0	9.6	-9.8
10	9	0	5.6	-5.7
10	9	2	7.7	7.4
10	9	3	6.0	5.4
10	10	0	3.7	3.9
10	10	1	2.9	2.4
10	10	2	1.6	2.2
10	10	3	1.5	1.2
10	11	0	2.5	2.2
10	11	1	1.6	-1.5
11	0	2	1.9	2.2
11	0	4	21.6	-23.2
11	0	6	1.5	-1.4
11	1	1	11.4	12.0
11	1	2	3.7	-4.2
11	1	3	11.3	-11.0
11	1	5	16.6	15.3
11	1	6	7.4	-6.8
11	1	7	3.6	-3.3
11	2	1	10.4	-10.2
11	2	2	22.0	-21.7
11	2	3	5.1	-4.4
11	2	4	16.2	14.9
11	2	6	4.7	3.9
11	2	7	4.7	-4.3
11	2	8	5.3	5.1
11	3	1	11.3	10.7
11	3	2	6.5	6.4
11	3	3	6.3	-6.5
11	3	4	4.4	4.2
11	3	5	2.9	2.4
11	3	6	9.6	-9.7
11	3	8	2.4	2.5
11	4	3	10.0	10.6
11	4	4	4.4	-5.0
11	4	5	2.9	-2.9
11	4	6	4.7	-4.6
11	4	7	4.7	3.7
11	4	8	4.7	4.5
11	5	1	5.8	-6.1
11	5	3	16.6	-17.4
11	6	1	7.9	-6.7
11	6	2	7.7	-8.2
11	6	3	13.0	13.4
11	7	1	11.2	11.5
11	7	3	3.9	1.9
11	8	1	2.9	-2.1
11	8	2	6.4	7.2
11	9	1	2.2	2.3
11	9	2	2.5	-2.4
11	10	2	3.6	-3.0
11	10	3	5.3	3.9
12	0	0	3.7	-3.9
12	0	2	6.2	5.2
12	0	6	2.5	2.6
12	1	0	10.4	-11.2
12	1	1	1.9	-1.5
12	1	2	18.6	17.3
12	1	3	3.0	2.6
12	1	6	2.1	-2.1
12	1	7	2.7	-2.2
12	2	0	10.6	-9.9
12	2	1	4.6	-5.0
12	2	2	10.4	-9.8
12	2	3	2.6	-2.1
12	2	4	2.7	-2.8
12	2	5	7.3	6.7
12	2	6	3.8	2.8
12	3	0	13.0	12.8
12	3	1	6.3	4.8
12	3	2	19.2	-19.1
12	3	3	9.5	-9.6
12	3	4	16.1	-16.5
12	3	5	5.1	5.4
12	3	6	3.8	3.9
12	3	7	2.1	-2.1
12	3	8	1.6	-1.8
12	4	0	7.8	-8.6
12	4	1	9.5	-9.3
12	4	2	6.5	7.3
12	4	3	3.5	-3.5
12	4	4	12.2	12.9
12	5	0	11.1	11.5
12	5	2	8.6	-7.8
12	5	3	2.4	-3.3
12	6	0	15.8	-15.1
12	6	3	2.4	2.0
12	7	0	24.9	23.6
12	7	1	17.5	-15.3
12	7	2	2.5	-3.1
12	8	0	10.6	-11.1
12	8	1	6.2	5.3
12	8	3	2.1	-1.7
12	9	0	10.1	-9.8
12	9	1	4.5	-4.5
12	9	2	2.9	-3.3
12	9	3	1.2	1.0
12	10	0	3.1	3.4
12	10	1	5.8	5.0
12	10	2	2.7	-2.0
13	0	2	10.8	9.9
13	1	1	1.8	-1.9
13	1	2	8.2	-8.8
13	1	3	6.7	-6.3
13	1	4	6.5	6.2
13	1	5	5.3	4.4
13	1	6	4.7	-4.8
13	1	7	6.3	-6.5
13	2	1	11.7	-11.4
13	2	2	12.2	-10.6
13	2	3	8.3	7.8
13	2	4	12.7	11.6
13	2	6	6.3	-5.3
13	2	7	2.1	-2.3
13	3	1	2.4	-2.3
13	3	4	8.0	8.8
13	3	6	3.8	-4.1
13	3	8	3.8	3.5
13	4	1	2.3	2.1
13	4	2	15.8	17.6
13	4	3	21.6	21.5
13	4	6	5.5	-5.7
13	4	8	2.9	2.7
13	5	1	6.8	6.2
13	5	2	6.4	-6.7
13	5	3	9.3	10.1
13	6	1	15.1	-15.5
13	6	2	9.5	9.8
13	7	1	3.0	-3.3
13	7	2	1.6	-1.3
13	8	1	5.6	5.5
13	8	2	13.7	13.7
13	9	1	3.5	-3.4
13	9	2	3.0	-3.1
13	9	3	1.1	0.9
13	10	1	1.6	1.7
14	0	0	14.0	-14.8
14	0	2	2.5	2.3
14	0	4	9.2	-10.7
14	1	0	4.5	-4.2
14	1	2	17.9	18.2
14	1	3	5.2	5.4
14	1	4	2.1	2.3
14	1	5	3.8	-4.4
14	1	8	2.9	2.8
14	2	0	26.7	28.0
14	2	1	11.9	10.9
14	2	2	9.1	8.4
14	2	3	5.0	-4.5
14	2	4	4.0	-3.6
14	2	6	5.3	5.0
14	3	0	14.0	13.6
14	3	1	8.2	7.3
14	3	3	7.1	-7.0
14	3	4	8.0	-9.1
14	3	6	4.0	4.3
14	3	8	2.7	2.6
14	4	1	5.9	5.9
14	4	2	6.3	-7.1
14	4	3	3.0	-2.1
14	4	4	6.3	-6.7
14	4	5	3.5	-2.8
14	4	6	3.5	-3.3
14	5	0	3.9	4.3
14	5	1	3.0	4.0
14	5	2	2.5	-3.2
14	5	3	9.3	-8.9
14	6	0	6.8	8.4
14	6	1	4.0	3.8
14	6	2	4.3	-4.5
14	7	0	6.6	7.1
14	7	1	7.4	-6.9
14	7	2	7.1	-7.7
14	8	0	9.8	8.9
14	8	1	5.8	5.7
14	8	2	5.6	5.8
14	8	3	2.8	-2.7
14	9	0	4.3	-4.3
14	10	0	4.1	4.4
14	10	1	2.3	2.5
15	0	2	16.1	-16.7
15	0	4	2.4	3.0
15	0	6	2.1	2.0
15	1	1	9.3	8.4
15	1	2	11.0	-11.7
15	1	4	6.5	5.8
15	1	5	7.1	6.9
15	2	1	7.1	-7.3
15	2	2	22.0	-23.1
15	2	3	4.7	4.4
15	2	4	14.2	12.5
15	2	7	3.3	-2.6
15	3	1	13.4	-13.9
15	3	2	7.1	-6.3
15	3	3	5.4	-5.9
15	3	5	3.3	-3.1
15	4	1	11.5	-10.7
15	4	2	3.9	-4.1
15	4	3	3.2	2.9
15	4	5	4.7	-4.6
15	5	2	7.7	-8.7
15	5	3	9.3	8.1
15	6	1	2.5	2.6
15	6	2	1.6	-2.0
15	6	3	9.8	9.9
15	7	1	7.1	-7.1
15	8	1	2.4	1.9
15	8	2	3.0	2.9
15	8	3	5.3	-4.7
15	9	2	2.4	-2.3
15	9	3	4.3	4.6
16	0	0	48.5	-50.7
16	0	2	12.1	10.9
16	0	6	6.3	-6.2
16	1	0	24.4	-25.1
16	1	1	6.5	6.5
16	1	2	4.3	-5.5
16	1	3	4.5	4.4
16	1	4	7.4	-7.6
16	1	5	5.5	-5.5
16	1	6	5.1	-4.9
16	2	0	12.1	-12.0
16	2	1	19.0	18.1
16	2	2	4.7	5.6
16	2	3	1.7	-2.1
16	2	4	2.9	3.6
16	3	0	3.5	3.8
16	3	1	12.3	10.8
16	3	2	4.5	4.7
16	4	1	12.4	12.2
16	4	2	4.1	3.5
16	4	4	7.7	7.5
16	4	5	4.4	-4.6
16	5	1	9.6	9.7
16	6	0	6.6	6.7
16	6	1	2.9	2.8
16	6	2	1.5	-2.4
16	6	3	1.6	1.6
16	7	2	3.0	-3.5
16	7	3	1.7	1.6
16	8	0	2.3	-2.0
16	8	1	1.7	1.6
16	8	3	1.7	-2.2
16	9	1	1.9	2.2
16	9	2	3.8	3.9
17	0	2	8.0	7.5
17	0	4	2.4	2.1
17	1	1	9.4	8.7
17	1	2	10.0	-9.5
17	1	3	14.0	-15.8
17	1	4	3.9	3.4
17	2	1	10.8	12.1
17	2	2	2.4	-2.2
17	2	3	5.3	5.7
17	2	4	5.1	4.1
17	2	5	3.5	3.7
17	2	6	3.8	-3.3
17	2	7	2.4	2.1
17	3	1	13.0	12.0
17	3	3	3.8	-3.2
17	3	6	2.7	2.4
17	3	7	2.1	2.6
17	4	1	3.0	-2.7
17	4	3	5.2	-5.5
17	4	5	4.4	-4.3
17	4	6	2.7	-2.1
17	5	2	5.0	-5.4
17	5	3	6.2	-5.4
17	6	3	1.4	1.6
17	7	1	4.3	3.5
17	7	2	2.3	2.0
17	7	3	1.6	-1.6
17	8	3	2.7	-2.9
18	0	0	17.2	-16.8
18	0	2	28.2	30.4
18	0	4	8.0	8.1
18	1	0	4.3	-4.3
18	1	1	9.1	-8.4
18	1	3	7.7	-6.8
18	1	5	3.9	3.8
18	2	0	13.2	-13.1
18	2	1	12.7	11.0
18	2	3	6.7	-6.4
18	2	4	4.7	-4.2
18	2	6	3.8	-3.3
18	3	1	4.3	-4.7
18	3	3	2.5	-2.5
18	3	4	3.8	3.4
18	3	8	4.7	4.4
18	4	0	5.6	-4.5
18	4	1	6.7	6.6
18	4	3	2.4	-2.1
18	4	5	2.1	-1.2
18	4	6	3.8	-4.7
18	5	1	2.8	-2.4
18	5	3	2.5	-2.4
18	6	0	7.4	6.7
18	7	1	2.8	-2.8
18	7	2	2.1	-1.8
18	7	3	1.7	1.8
19	0	2	13.2	13.3
19	0	4	5.8	-5.7
19	1	1	3.9	-3.6
19	1	2	3.9	-3.6
19	1	3	3.1	-2.7
19	1	4	7.1	6.5
19	1	5	5.4	5.5
19	2	1	3.7	-3.4
19	2	2	5.8	5.6
19	2	3	8.4	-8.4
19	2	4	5.3	-5.3
19	2	5	2.9	-2.9
19	2	6	2.4	-2.2
19	3	2	2.5	1.7
19	3	3	3.7	3.4
19	3	5	3.1	3.3
19	3	6	2.9	-2.9
19	4	1	4.9	4.8
19	4	2	2.2	2.5
19	4	3	2.1	-1.7
19	5	1	5.4	-5.0
19	5	2	2.1	-2.4
19	6	2	2.5	-2.2
19	6	3	1.6	1.7
19	7	2	1.6	1.8
20	0	0	11.9	-11.6
20	0	2	4.1	4.5
20	0	4	7.4	-8.0
20	0	6	1.8	-2.2
20	1	0	4.1	4.1
20	1	2	2.4	2.9
20	1	3	1.5	0.6
20	1	4	3.6	3.9
20	1	5	1.8	2.2
20	2	0	6.9	6.1
20	2	1	5.2	5.2
20	2	3	5.8	-5.6
20	2	4	4.0	-4.5
20	2	6	1.6	1.3
20	3	2	3.9	-3.4
20	3	3	2.4	2.5
20	4	0	2.6	3.2
20	4	1	4.3	3.9
20	4	4	3.5	2.9
20	4	5	1.6	1.7
20	5	3	3.9	4.1
20	6	0	4.7	4.4
20	6	3	1.2	-1.4
20	7	0	1.5	1.6
21	0	4	4.7	-5.2
21	1	1	2.1	1.4
21	1	2	2.2	-2.6
21	1	4	6.3	5.8
21	1	5	3.5	3.2
21	2	1	3.9	3.7
21	2	2	2.2	1.8
21	2	5	2.4	2.1
21	3	5	2.7	-2.7
21	4	1	4.7	4.0
21	4	2	3.2	-3.1
21	4	3	2.8	-2.7
21	5	1	1.7	1.7
21	5	2	2.5	-2.5
21	6	1	2.3	-1.3
21	6	2	3.6	-3.7
22	0	0	3.3	-2.7
22	0	2	4.3	4.7
22	1	2	2.1	-1.3
22	2	0	3.7	3.1
22	2	3	3.7	-3.4
22	3	1	2.3	-1.9
22	3	3	1.5	-1.2
22	4	0	6.7	-5.7
22	4	2	2.4	-2.3
22	4	3	1.6	-2.0
22	4	4	1.5	1.5
22	5	0	3.0	-3.1
22	6	0	3.1	-3.6
23	0	2	2.1	-1.7
23	1	2	3.5	-3.2
23	1	3	3.0	-3.1
23	2	1	3.7	-3.0
23	2	2	2.1	1.8
23	2	3	1.6	-1.8
23	3	2	2.9	2.0
23	3	3	0.6	-0.5
24	0	0	5.0	-5.0
24	1	0	3.6	3.6
24	1	3	1.8	2.2
24	2	0	1.8	2.4
24	3	1	1.4	-1.7

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	Mean isotropic $B=5·04$					
H(4)	0·2250	0·1404	−0·0344						
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

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On the crystal structures of some α-oxoacids*

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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.

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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