These pairs of HPO$_4^{2-}$ ions lie in sheets parallel to the (100) plane (Fig. 1). The tin(II) ions are in sheets midway between the phosphate sheets. Each tin(II) ion has a total of eight oxygen neighbors from a total of six different phosphate ions (Fig. 3). Of these eight neighbors, three are at an average distance of 2·26 Å, two are at an average distance of 2·66 Å, and three are at an average distance of 3·27 Å. Each oxygen atom has two Sn neighbors.

In SnHPO$_4$ the hydrogen bonds join pairs of phosphate ions. This differs from structures such as H$_3$PO$_4$ (Smith, Brown & Lehr, 1955) and KH$_2$PO$_4$ (Frazer &
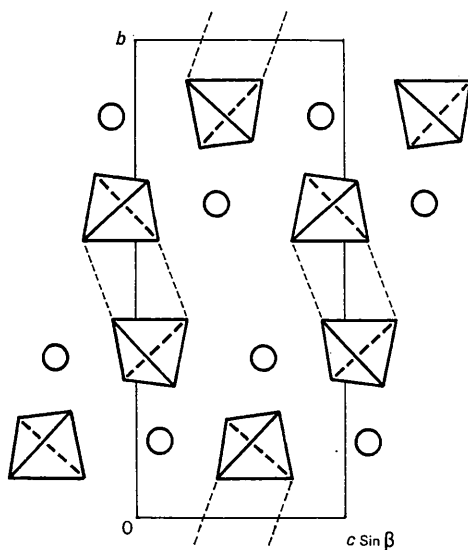

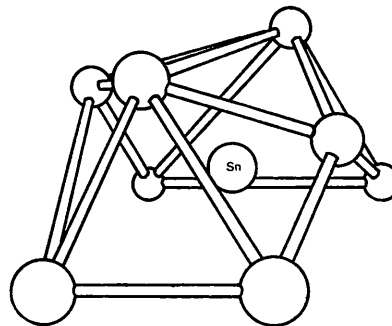
Fig. 3. Isometric drawing of the configuration of oxygen atoms about an Sn(II)ion. The twofold screw axis is vertical.

Pepinsky, 1953; Levy, Petersen & Simonsen, 1953) in which there are a sufficient number of hydrogen bonds to form continuous two- or three-dimensional networks of phosphate ions.

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Fig. 2. Projection of the structure down the [100] axis.

A Refinement of the Structure of Rhombohedral Acetamide

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A more accurate analysis of the structure of rhombohedral acetamide using counter measured intensities has shown the earlier determination to be correct. The principal bond distances found are, C–C 1·530 (5), C–N 1·338 (7) and C–O 1·258(6) Å.

The structure of rhombohedral acetamide was determined by Senti & Harker (1940) using three-dimensional Patterson syntheses and partially refined with the aid of two- and three-dimensional F_o syntheses. Although the interatomic distances reported by Senti & Harker do

not differ greatly from those determined more recently in orthorhombic acetamide (Hamilton, 1965) and in other related amides, because of the limited techniques available to the early workers in 1940, reliable quantitative comparison with the published work on rhombohedral acetamide is not possible. It was considered timely, therefore, to confirm the original determination of this structure and to refine the structural parameters using

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counter-measured data and least-squares refinement techniques.

Experimental

Suitable evenly developed crystals were grown by slowly cooling a saturated solution of acetamide in ethyl acetate from 35 °C to room temperature; the addition of 10% of ethanol with stirring was found to inhibit the formation of the fine acicular habit. The crystals so obtained exhibited the forms {10.0} and {11.3}. Rapid deterioration of the faces occurred on exposure to air, for rhombohedral acetamide is markedly hygroscopic.

The crystal selected for intensity measurements was sealed in a Lindemann glass tube of wall thickness 0·1 mm; it was approximately equidimensional with maximum and minimum 'diameters' of 0·34 mm and 0·46 mm respectively. Using Cu $K\alpha$ radiation ($\lambda = 1·5418$ Å) the cell dimensions were determined at two temperatures using a least-squares fit of θ values of reflexions. The three circle diffractometer (Small & Travers, 1961) was used for the measurement of θ values. The unit-cell dimensions and standard deviations based on a hexagonal unit cell together with those recorded by Senti & Harker are shown in Table 1.

Table 1. *Cell dimensions*

		a	c
Senti & Harker		11·44 (3) Å	13·49 (3) Å
Denne & Small	298°K	11·526 (5)	13·589 (5)
Denne & Small	173°K	11·536 (5)	13·194 (5)

Weissenberg photographs indicated a rhombohedral lattice with reflecting conditions $(-h+k+l) = 3n$ for $hk.l$ and $l=2$ for $h\bar{h}.l$; a pyroelectric test was positive, thus confirming the space group $R3c$ found by the previous workers.

Using the three-circle diffractometer, and the procedure previously described (Hughes & Small, 1962) the intensities of 399 reflexions were measured; to improve the mosaicity of the crystal used, it had previously been dipped in liquid nitrogen. Corrections for the absorption of X-rays by the enclosing Lindemann glass tube were applied to the measured intensities. Absorption within the crystal was allowed for on the assumption that its shape aproximated to a sphere. Intensities were reduced to an approximate absolute scale by the statistical method of Wilson. An $N(z)$ *versus* z test (Howells, Phillips & Rogers, 1950) for centrosymmetry was, unexpectedly, positive. An inspection of the structural arrangement reported by Senti & Harker suggested an explanation of this result. Pairs of molecules

were noted to be related by a pseudo-centre of symmetry arising from the similarity in scattering power of oxygen and nitrogen atoms. The difference in charge and polarizability of the NH_2 group and the oxygen atom leaves the structure with a detectable pyroelectric effect.

Refinement of the structure determination

Using the atomic coordinates reported by Senti & Harker and an overall isotropic temperature factor (B value) of 4·2, a set of structure factors for all unique reflexions to the limit of observation was calculated, the agreement index R was found to be 0·387. For this and all subsequent structure factor calculations the atomic scattering factors listed in *International Tables for X-ray Crystallography* (1962) were used. A least-squares refinement of the positional coordinates of oxygen, nitrogen and carbon atoms and their anisotropic temperature factors was carried out initially using the block-diagonal least-squares program *SFLS* written by J. S. Rollett for the MERCURY computer. Refinement was slow and after eighteen cycles R had decreased to only 0·136. This slow convergence was attributed to neglect of off-diagonal terms in the normal least-squares matrix between some of which strong correlation arose from the pseudo-centre of symmetry.

Later refinement employed the full-matrix program *ORFLS* of Busing, Martin & Levy (1962) as adapted for the X-ray 63 *System* on the ATLAS computer at Chilton. An $(F_o - F_c)$ Fourier synthesis showed the five hydrogen atoms near their expected positions, they were given b_{ij} values identical to those of the atoms to which they were attached and were included but not refined in the least-squares refinement. At this point in the refinement it was noted that the calculated structure factors of the two strongest reflexions, 110 and 113, had magnitudes substantially greater than those observed. It was concluded that these observed structure factors were likely to be affected by systematic errors due to extinction, and they were therefore omitted from the succeeding refinement cycles.

Table 2. *Fractional atomic coordinates*

		x	y	z
C(1)	(methyl)	0·4767 (4)	0·1255 (5)	0·0333 (5)
C(2)		0·3403 (3)	0·0006 (4)	0·0391 (5)
O		0·2417 (3)	−0·0039 (4)	−0·0014 (−)
N		0·3320 (5)	−0·1007 (4)	0·0909 (3)
H(1)	(amide)	0·244 (6)	−0·170 (6)	0·099 (4)
H(2)	(amide)	0·409 (6)	−0·100 (5)	0·117 (4)
H(3)		0·470 (6)	0·202 (5)	0·086 (4)
H(4)		0·527 (6)	0·087 (5)	0·040 (5)
H(5)		0·482 (6)	0·189 (5)	−0·021 (4)

Table 3. b_{ij} *values*

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(1)	0·0084 (4)	0·0095 (5)	0·0081 (3)	0·0018 (4)	0·0000 (4)	0·0003 (4)
C(2)	0·0074 (4)	0·0083 (4)	0·0054 (2)	0·0032 (3)	0·0001 (3)	−0·0010 (3)
O	0·0092 (3)	0·0088 (3)	0·0084 (2)	0·0041 (3)	−0·0018 (2)	0·0003 (2)
N	0·0087 (4)	0·0094 (4)	0·0070 (2)	0·0037 (4)	−0·0005 (3)	0·0009 (3)

In the last two cycles of least-squares refinement the hydrogen atom positions were also refined. An R value of 0·045 was reached when the shifts in the parameters of the heavy atoms were less than one tenth of their standard deviations. The atomic coordinates are listed in Table 2 and the b_{ij} values are given in Table 3. For each atom the root mean square displacements parallel to the principal axes of the vibration ellipsoids are listed in Table 4. It was noted that the average displacement of the central carbon atom has the lowest value and that its vibration is relatively isotropic. A simple vibrational model with the other three atoms 'riding' on the central carbon was therefore used as the basis of the corrections to bond distance for librational motion. The bond distances before and after application of these corrections are shown in Table 5 and the bond angles are listed in Table 6. The 'best' plane through the atoms C(1), C(2), O and N was determined by least squares and the parameters of this plane with the distance of all atoms from it are given in Table 7. A list of observed and calculated structure factors is given in Table 10.

Table 4. Root mean square displacement along ellipsoid axes

C(1)	0·189 (5) Å	0·267 (6) Å	0·277 (7) Å
C(2)	0·191 (5)	0·202 (5)	0·239 (4)
O	0·205 (4)	0·211 (4)	0·293 (4)
N	0·207 (5)	0·220 (5)	0·268 (5)

Table 5. Bond distances

	Before libration correction	After libration correction
C——C	1·513 (5) Å	1·530 (5) Å
C——N	1·324 (6)	1·338 (7)
C——O	1·241 (6)	1·258 (6)
N——H(1)	0·93 (8)	
N——H(2)	0·96 (8)	
C(1)–H(3)	1·25 (8)	
C(1)–H(4)	0·90 (8)	
C(1)–H(5)	1·02 (8)	

Table 6. Bond angles

C(1)	C(2)	N	116·7 (5)°
C(1)	C(2)	O	120·7 (5)
N	C(2)	O	122·6 (5)
C(2)	N	H(1)	113 (4)
C(2)	N	H(2)	122 (3)
H(1)	N	H(2)	124 (5)

Table 7. Deviations of atoms from the 'best' plane (referred to orthogonal axes a,b',c)

$$-0.4337x + 0.3571y + 0.8273z = -1.2502$$

C(1)	0·0022 Å	H(1)	0·102 Å
C(2)	−0·0075	H(2)	−0·089
N	0·0025	H(3)	1·170
O	0·0028	H(4)	−0·395
		H(5)	−0·266

Discussion of the structure

The positional parameters obtained from this investigation differ by as much as 0·2 Å from those of Senti & Harker. The agreement between the bond distances is however remarkable, the differences between the C–C, C–N and C–O bond distances found in the two determinations are only 0·02 Å, 0·04 and 0·02 respectively. The present authors find the accuracy of the original determination, in the context of its time, quite impressive.

A reminder of the well known structural arrangement in rhombohedral acetamide is given in Fig. 1. The arrangement, which is unique amongst amides so far reported, exhibits maximum hydrogen bonding with each molecule donating two hydrogen bonds and accepting two; the distances involved in these bonds are given in Table 8. The closest intermolecular approaches not involved in hydrogen bonding are between hydrogen atoms in neighbouring molecules; 2·64(10) Å between H(5) and H(2) and 2·73(10) between H(4) and H(3); both are in excess of the sum of the accepted values of the van der Waals radii (Bondi, 1964).

Table 8. Hydrogen bond distances

N–H(1)–O	2·951 (6) Å	H(1)–(N–O line)	0·26 (7) Å
N–H(2)–O	2·910 (8)	H(2)–(N–O line)	0·05 (7)

Molecules related by the c-glide plane are also related by the pseudo-centre of symmetry referred to previously. Table 9(a) gives the coordinates of the molecule related by c-glide to the molecule defined in Table 2; for comparison, in Table 9(b) are the coordinates of a molecule related by a centre of symmetry at $(\frac{2}{3},\frac{1}{3},0\cdot290)$. The correspondence, with interchange of O and N, will be seen to be close enough to explain the observed centricity of the diffracted intensity distribution.

A full discussion of the interatomic distances and molecular arrangement in comparison with those in orthorhombic acetamide (Hamilton, 1965), monofluo-

Table 9. Fractional coordinates

	(a) Molecule related by c-glide				(b) Molecule related by pseudo-centre		
	x	y	z		x	y	z
C(1)	0·874	0·523	0·533	C(1)	0·856	0·541	0·547
C(2)	0·999	0·660	0·539	C(2)	0·993	0·666	0·541
O	0·004	0·758	0·499	N	0·001	0·767	0·489
N	0·101	0·668	0·591	O	0·091	0·671	0·581

Table 10. *Observed and calculated structure factors*

H	K	L	FO	FC	A	B
0	0	6	64.08	65.20	23.66	60.75
0	0	12	15.85	16.40	2.65	15.19
0	1	2	24.77	23.48	21.48	-0.49
0	1	8	8.14	7.88	-7.87	-0.31
0	1	14	8.14	8.54	7.34	-4.36
0	2	4	49.43	47.36	-12.98	45.54
0	2	10	13.87	14.48	-14.08	-3.36
0	2	16	2.76	2.69	-2.60	0.69
0	3	0	69.51	72.67	72.26	7.74
0	3	6	24.63	26.74	-1.02	26.72
0	3	12	9.32	8.93	-8.90	-0.74
0	4	2	104.29	104.22	95.28	-42.23
0	4	8	5.73	7.18	5.99	3.95
0	4	14	13.06	14.50	13.74	-4.00
0	5	4	51.56	52.56	20.12	-48.56
0	5	10	19.13	20.02	16.76	10.95
0	5	16	1.55	2.21	1.94	-1.06
0	6	0	22.44	21.74	21.72	0.75
0	6	6	29.46	30.11	0.52	30.10
0	6	12	16.63	17.24	-17.17	1.54
0	7	2	14.01	14.40	1.44	-14.42
0	7	8	12.88	12.74	9.30	-8.71
0	7	14	2.10	1.83	1.34	1.25
0	8	4	25.46	25.20	24.78	-4.59
0	8	10	10.50	10.55	3.54	9.04
0	9	0	46.66	47.37	47.35	-1.52
0	9	6	13.75	13.35	-1.13	13.30
0	9	12	3.34	4.47	-0.54	4.44
0	10	2	10.93	10.63	-10.23	2.90
0	10	8	5.03	6.29	-5.60	-2.85
0	11	4	4.00	4.04	3.99	0.67
0	12	0	18.87	18.33	18.00	3.47
1	0	4	88.24	90.00	34.93	-82.94
1	0	10	20.06	19.94	17.89	8.80
1	0	16	2.16	2.69	2.69	0.13
1	1	6	25.72	20.56	-8.65	-18.66
1	1	9	14.82	14.97	-7.43	12.99
1	1	12	5.01	3.34	0.85	-3.23
1	1	15	7.22	7.56	1.70	-7.37
1	2	2	35.47	34.50	-34.32	3.55
1	2	5	58.11	56.68	-27.89	49.35
1	2	8	8.89	9.77	7.45	-6.32
1	2	11	19.97	19.66	19.03	4.93
1	2	14	6.10	6.96	-5.76	3.90
1	2	17	3.48	4.08	-1.48	3.80
1	3	1	32.57	31.13	30.12	-7.84
1	3	4	24.48	23.85	19.67	-13.48
1	3	7	16.63	16.53	0.64	16.51
1	3	10	7.22	8.18	6.37	5.14
1	3	13	2.22	2.15	-2.15	-0.11
1	3	16	1.61	1.81	1.58	-0.87
1	4	0	62.98	65.06	64.75	-6.35
1	4	3	28.63	27.35	-20.99	17.53
1	4	6	9.75	5.89	3.83	-4.47
1	4	9	19.71	18.92	-11.18	-15.26
1	4	12	12.46	12.98	12.12	4.66
1	4	15	7.28	7.30	5.07	-5.26
1	5	2	33.06	31.82	-26.09	18.22
1	5	5	41.72	35.33	3.72	35.13
1	5	8	10.67	11.02	-11.02	-0.12
1	5	11	10.53	10.14	6.19	8.03
1	5	14	2.62	2.53	-1.64	-1.93
1	6	1	15.54	15.51	-7.81	13.40
1	6	4	15.56	14.97	-9.69	11.41
1	6	7	34.12	33.66	2.38	33.58
1	6	10	8.14	7.83	-4.84	-6.16
1	6	13	1.41	1.40	0.20	-1.38
1	7	3	32.02	32.22	-21.73	23.79
1	7	6	15.16	14.98	-2.48	-14.77
1	7	0	13.21	13.15	-11.36	6.63
1	7	9	11.13	11.48	-9.80	-5.98
1	7	12	6.62	7.20	6.24	-3.58
1	8	2	19.07	19.57	17.27	-9.19
1	8	8	5.06	4.88	2.44	4.22
1	8	5	10.62	10.28	6.88	-7.63
1	8	11	2.99	2.26	2.19	0.59
1	9	1	13.55	13.87	-2.36	13.67
1	9	4	9.24	8.79	-4.72	-7.41
1	9	7	9.49	8.68	-3.62	7.89
1	9	10	2.91	3.13	3.09	0.53
1	10	0	13.09	12.50	-12.31	-2.17
1	10	3	19.05	18.52	-14.82	11.12
1	10	6	1.87	1.94	0.96	-1.69
1	10	9	2.24	2.57	1.04	2.35
1	11	2	2.33	1.35	1.33	-0.19
1	11	5	3.05	3.51	-0.44	3.48
1	12	1	2.36	2.28	2.24	-0.45
2	0	2	47.79	48.15	-34.68	33.41
2	0	8	6.21	6.23	-1.45	6.06
2	0	14	6.30	6.44	-6.20	1.73
2	1	1	29.17	29.10	23.80	-16.74
2	1	4	68.73	68.77	-38.19	57.19
2	1	7	86.11	80.61	20.08	78.07
2	1	10	16.08	16.87	-13.46	-10.14
2	1	13	4.86	5.07	-2.03	4.64
2	1	16	2.07	2.07	-2.07	0.18
2	2	0	119.02	120.49	-120.49	-0.00
2	2	3	19.85	17.55	-16.94	4.57
2	2	6	25.86	24.40	-8.92	-22.91
2	2	9	16.00	16.09	9.08	13.29
2	2	12	5.06	5.09	1.48	-4.87
2	2	15	5.75	6.09	-5.47	2.67
2	3	2	26.55	27.27	-23.70	13.48
2	3	5	52.79	52.88	18.83	-49.41
2	3	8	4.29	4.16	-4.14	0.38
2	3	11	7.97	8.16	-7.04	-4.12
2	3	14	4.06	4.07	-3.86	1.30
2	4	1	18.07	15.82	-5.90	14.68
2	4	4	21.43	19.83	-17.15	9.97
2	4	7	13.23	13.46	-6.75	-11.65
2	4	10	5.96	6.08	-4.03	-4.55
2	4	13	0.92	0.80	0.89	0.07
2	5	0	53.57	53.23	-53.21	-1.66
2	5	3	6.99	6.79	-4.18	5.35
2	5	6	11.02	11.44	1.05	-11.39
2	5	9	30.15	29.30	20.69	20.74
2	5	12	2.65	2.25	1.36	-1.79
2	5	15	5.98	6.61	-3.89	5.35
2	6	2	11.48	11.26	-8.42	7.47
2	6	5	13.06	12.85	-11.89	4.86
2	6	8	2.93	2.06	0.45	2.01
2	6	11	6.10	6.01	4.92	-3.45
2	6	14	4.78	4.24	-3.87	1.73
2	7	1	22.99	24.63	16.75	-18.06
2	7	4	11.02	10.91	-7.52	7.90
2	7	7	11.85	11.50	7.52	-8.70
2	7	10	3.74	3.58	-3.12	-1.75
2	7	13	3.91	4.22	-3.20	2.75
2	8	0	18.50	18.18	-18.14	-1.11
2	8	3	19.36	20.05	13.74	-14.60
2	8	6	3.19	2.83	-0.78	-2.72
2	8	9	4.06	4.55	4.55	0.05
2	8	12	1.55	1.02	0.98	-0.26
2	9	2	10.41	10.85	-6.08	8.98
2	9	5	15.28	15.32	-0.61	15.31
2	9	8	3.02	2.67	-2.42	1.12
2	10	1	4.37	4.06	-3.37	-2.27
2	10	4	6.01	5.35	-4.39	3.05
2	10	7	7.42	7.32	0.35	7.31
2	11	0	11.71	10.88	-10.88	0.43
2	11	3	8.06	8.08	4.94	-6.40
3	0	0	67.78	72.67	72.26	-7.74
3	0	6	35.21	35.85	24.52	26.16
3	0	12	6.53	6.39	-5.68	2.73
3	1	2	46.55	46.73	43.09	-18.08
3	1	5	17.41	17.99	-17.67	-3.37
3	1	8	3.37	4.97	2.86	4.07
3	1	11	5.55	5.60	3.59	-4.30
3	1	14	3.05	3.16	3.10	-0.40
3	2	1	26.04	26.86	13.62	-23.15
3	2	4	17.95	16.93	-9.88	13.74
3	2	7	45.20	43.20	-3.91	-43.02
3	2	10	10.10	9.81	-9.43	-2.69
3	2	13	1.44	1.80	-1.59	-1.02
3	2	16	2.01	1.90	-1.87	0.32
3	3	0	13.03	12.36	-12.36	0.00
3	3	3	73.10	73.66	50.01	-54.07
3	3	6	21.66	21.37	-2.37	21.24
3	3	9	17.78	19.10	-5.38	-18.33
3	3	12	16.80	17.06	-17.01	-1.38
3	3	15	3.57	3.58	3.20	1.61
3	4	2	16.86	17.52	17.07	-3.97
3	4	5	7.85	8.38	3.33	7.69
3	4	8	7.97	8.86	8.54	2.34
3	4	11	6.62	6.07	-5.50	2.56
3	4	14	1.75	1.38	0.12	1.37
3	5	1	11.41	10.88	-9.31	-5.64
3	5	4	4.06	4.32	3.99	1.67
3	5	7	6.53	7.14	-1.12	7.05
3	5	10	5.15	1.67	-1.12	1.24
3	5	13	1.08	1.13	-0.84	-0.76
3	6	0	10.01	10.82	9.78	-4.62
3	6	3	6.36	4.81	3.80	-2.94
3	6	6	14.04	15.74	1.48	15.67
3	6	9	11.77	12.01	-9.70	-7.08
3	6	12	8.60	9.14	-8.76	2.61
3	7	2	16.46	17.70	-16.41	6.62
3	7	5	23.07	23.30	4.68	-22.91
3	7	8	4.95	4.83	-1.87	-4.45
3	7	11	6.67	6.00	-4.64	-3.80
3	8	1	8.11	8.77	-4.04	7.78
3	8	4	5.90	6.51	3.07	5.74
3	8	7	9.47	8.99	-4.60	-7.72
3	8	10	2.42	3.10	-2.82	-1.29
3	9	0	14.59	14.71	14.69	-0.67
3	9	3	2.96	3.44	-2.61	-2.24
3	9	6	5.78	5.59	2.49	5.01
3	9	9	2.59	2.51	2.13	1.34
3	10	5	4.46	4.68	-2.27	-4.10
4	0	4	86.48	86.40	49.27	-71.09
4	0	10	29.43	30.00	27.75	11.41
4	0	16	5.44	6.13	5.62	-2.45
4	1	0	64.07	65.06	64.75	6.35
4	1	3	34.67	33.52	-11.43	31.52
4	1	6	7.02	7.78	1.40	-7.65
4	1	9	18.33	17.38	-15.46	-7.77
4	1	12	10.79	11.53	10.89	3.80
4	1	15	4.03	5.35	2.30	-4.83
4	2	2	36.05	33.86	-33.76	2.59
4	2	5	6.44	3.90	3.73	-1.43
4	2	8	9.26	8.56	-1.93	-8.34
4	2	11	6.34	6.11	-6.11	-0.10
4	2	14	2.88	2.94	-2.74	1.08
4	3	1	17.41	16.37	-13.03	9.90
4	3	4	9.35	9.21	8.29	4.02
4	3	7	16.46	16.89	-5.88	-15.84
4	3	10	1.64	2.84	-0.71	-2.75
4	3	13	4.29	4.42	3.94	-2.01
4	4	0	47.53	44.89	44.89	-0.00
4	4	3	16.46	15.83	-12.70	9.45
4	4	6	18.73	20.58	6.38	-19.55
4	4	9	9.12	9.27	-7.64	-5.26
4	4	12	16.74	17.31	17.28	1.07
4	5	2	21.78	22.65	20.90	-8.72
4	5	5	4.80	4.56	-1.84	-4.17
4	5	8	6.10	6.48	-3.73	5.30
4	5	11	1.27	0.87	0.32	-0.81
4	6	1	3.14	2.48	0.83	-2.34
4	6	4	10.36	11.23	-4.90	-10.18
4	6	7	7.11	7.33	0.81	-7.29
4	6	10	3.45	3.74	2.48	-2.88
4	7	0	5.75	6.73	-6.55	1.55
4	7	3	5.01	5.37	2.39	4.88
4	7	6	7.37	7.37	1.31	-7.25
4	7	9	6.44	5.75	-5.01	-2.81
4	8	2	20.94	21.13	18.18	-10.76
4	8	5	2.59	3.14	2.28	2.16
4	8	8	5.32	6.04	5.97	0.93
4	9	1	2.62	2.87	-2.51	1.40
4	9	4	6.53	6.33	2.31	-5.89
4	9	7	1.96	2.15	-1.51	-1.53
4	10	0	3.25	3.63	-2.80	-2.31
4	10	3	6.82	6.64	-2.11	6.30
5	0	2	21.63	23.80	23.22	-5.21
5	0	8	11.91	11.71	-10.33	5.52
5	0	14	7.91	9.43	7.70	-5.45
5	1	1	16.25	17.45	-13.44	11.13
5	1	4	5.70	6.26	-3.38	-5.27
5	1	7	24.08	24.34	10.77	21.82
5	1	10	3.24	3.48	1.43	3.17
5	1	13	3.34	3.74	2.63	2.65
5	2	0	54.17	53.23	-53.21	1.66
5	2	3	8.03	7.47	5.30	5.26
5	2	6	15.25	13.93	-8.11	-11.32
5	2	9	29.20	31.50	19.46	24.89
5	2	12	4.75	5.00	-1.34	-4.91
5	2	15	6.10	6.63	-4.11	5.21
5	3	2	32.60	26.32	22.62	-13.46
5	3	5	3.19	3.52	-0.77	3.44
5	3	8	6.07	6.80	6.43	2.23
5	3	11	3.19	2.62	2.59	0.40
5	3	14	2.50	2.95	2.95	-0.02
5	4	1	8.60	9.18	8.72	-2.88
5	4	4	19.25	19.71	11.49	-16.01
5	4	7	4.63	4.65	3.14	3.44
5	4	10	14.30	13.76	9.64	9.82
5	4	13	2.04	2.40	-1.16	2.10
5	5	0	1.61	2.91	2.91	-0.00
5	5	3	3.60	4.24	4.22	0.38
5	5	6	5.38	5.65	-3.32	4.57
5	5	9	16.08	16.23	11.10	11.85
5	5	12	2.47	2.32	1.00	2.18
5	6	2	13.90	14.20	-12.90	5.94
5	6	5	17.12	18.65	-6.66	17.42
5	6	8	4.86	5.40	-3.31	-4.27
5	6	11	2.88	3.08	2.49	1.82
5	7	1	4.00	4.52	-0.06	-4.52
5	7	4	6.16	6.79	6.45	2.18
5	7	7	3.88	4.53	3.15	3.24
5	7	10	0.92	1.36	0.39	1.30
5	8	0	5.67	6.32	4.66	4.27
5	8	3	7.65	7.69	5.12	-5.74
5	8	6	6.39	6.55	-4.00	-5.19
5	9	2	2.01	2.26	1.55	-1.65
6	0	0	22.41	21.74	21.72	-0.75
6	0	6	35.90	37.09	0.63	37.08
6	0	12	14.59	14.91	-14.43	3.76
6	1	2	28.86	29.28	-25.17	14.96
6	1	5	38.26	37.95	-17.75	33.55
6	1	8	2.47	3.06	-0.04	-3.06
6	1	11	7.88	7.64	7.55	1.13
6	1	14	1.27	4.28	-4.08	1.29
6	2	1	4.86	4.39	4.31	-0.87
6	2	4	19.33	19.37	-6.85	18.11
6	2	7	18.99	19.00	1.78	18.91
6	2	10	9.35	9.07	-8.73	-2.45
6	2	13	3.48	3.37	-3.12	-1.26
6	3	0	10.76	10.82	9.78	4.62
6	3	3	10.96	10.87	-3.37	-10.34
6	3	6	20.28	20.03	-4.00	19.62
6	3	9	14.50	14.84	-7.28	-12.94
6	3	12	9.55	9.72	-9.65	1.14
6	4	2	17.72	18.24	-16.87	6.93
6	4	5	7.25	7.49	6.48	-3.76
6	4	8	4.95	4.74	-4.52	-1.41
6	4	11	1.15	1.12	-0.02	1.12
6	5	1	12.28	12.38	-7.56	9.81
6	5	4	6.27	5.92	-4.04	4.32
6	5	7	14.10	13.18	-2.92	12.85
6	5	10	2.30	2.87	-2.42	-1.55
6	6	0	2.42	2.18	-2.18	-0.00
6	6	3	9.06	9.12	-8.52	3.26
6	6	6	8.83	8.54	0.90	8.49
6	6	9	4.89	4.53	2.93	3.45
6	7	2	4.63	4.90	-4.38	-2.19
6	7	5	7.39	7.22	0.08	-7.22
6	7	8	2.53	2.74	2.73	-0.09
6	8	1	5.18	5.29	4.98	1.79
6	8	4	4.60	4.89	-0.63	4.85
7	0	4	7.74	6.51	-6.43	1.00
7	0	10	6.70	6.56	0.77	-6.52
7	1	0	12.92	13.15	-11.36	-6.63
7	1	3	40.10	38.58	-29.27	25.14
7	1	6	20.37	19.38	5.98	-18.43
7	1	9	12.11	12.04	-10.99	-4.90
7	1	12	7.97	7.93	7.80	-1.41
7	2	2	9.15	9.40	-9.48	0.43
7	2	5	25.69	25.75	6.23	-24.98
7	2	8	2.99	2.91	0.16	-2.91
7	2	11	3.14	3.27	-0.43	-3.24
7	3	1	9.38	8.86	8.84	-0.52
7	3	4	6.47	6.70	-5.94	3.28
7	3	7	19.25	19.08	-3.59	-18.74
7	3	10	4.34	4.51	-1.12	-4.37
7	4	0	5.93	6.73	-6.55	-1.55
7	4	3	4.46	4.03	-3.02	2.68
7	4	6	7.42	7.30	3.90	-6.17
7	4	9	7.68	7.47	-4.54	-5.93
7	5	2	7.85	8.38	8.26	1.39
7	5	5	6.07	6.31	-1.47	6.13
7	5	8	2.13	2.26	1.46	1.72
7	6	1	4.63	4.89	0.50	-4.86
7	6	4	5.55	6.07	-5.77	1.90
7	6	7	2.93	3.36	-0.51	-3.32
7	7	0	10.87	11.97	-11.97	-0.00
7	7	3	1.96	1.80	-0.76	1.73
8	0	2	49.92	52.52	51.37	-10.96
8	0	8	12.23	11.83	4.35	11.00
8	1	1	7.80	7.56	1.79	-7.34
8	1	4	9.09	9.21	5.77	-7.17
8	1	7	5.09	5.28	5.16	1.16
8	1	10	4.23	4.13	2.28	3.44
8	2	0	18.38	18.18	-18.14	1.11
8	2	3	22.61	21.08	18.28	-10.50
8	2	6	6.65	6.23	-2.91	-5.51
8	2	9	4.86	4.65	3.84	2.62
8	2	12	0.92	1.89	-0.68	-1.77
8	3	2	5.73	5.30	5.30	0.09
8	3	5	3.74	3.93	3.37	-2.02
8	3	8	2.10	2.43	1.89	-1.52
8	3	11	3.65	2.85	-2.61	1.13
8	4	1	2.56	2.72	-2.67	-0.52
8	4	4	7.11	7.55	6.19	-4.33
8	4	7	2.73	2.69	0.52	-2.64
8	5	0	5.70	6.32	4.66	-4.27
8	5	3	5.73	5.83	3.69	-4.51
8	5	6	8.77	8.49	0.92	-8.44
8	6	2	1.15	1.46	0.37	1.41
8	6	5	5.61	5.50	-0.18	-5.59
9	0	0	46.69	47.37	47.35	1.52
9	0	6	16.86	14.77	1.03	14.74
9	0	12	5.18	5.40	0.67	5.35
9	1	2	9.04	10.11	-10.09	-0.62
9	1	5	15.02	14.46	-7.85	12.14
9	1	8	3.71	3.35	-3.33	-0.41
9	2	1	8.52	8.01	-7.38	3.09
9	2	4	4.69	4.71	0.42	4.69
9	2	7	3.65	4.33	-0.59	4.29
9	2	10	2.88	3.31	-3.18	-0.94
9	3	0	14.99	14.71	14.69	0.67
9	3	3	5.29	4.95	4.40	-2.26
9	3	6	5.26	4.87	1.11	4.74
9	3	9	4.09	3.86	2.55	2.90
9	4	2	13.29	13.15	11.34	-6.66
9	4	5	1.21	0.86	-0.72	0.47
9	5	1	1.78	2.74	0.82	2.61
9	5	4	1.96	1.65	-1.41	-0.86
10	0	4	6.36	6.02	-2.71	-5.37
10	0	10	6.04	5.35	5.04	1.79
10	1	0	13.09	12.50	-12.31	2.17
10	1	3	19.42	18.97	-11.20	15.32
10	1	6	2.16	2.26	-1.99	1.07
10	1	9	5.49	5.72	0.26	5.72
10	2	2	8.31	8.29	-8.23	0.97
10	2	5	8.14	8.57	-4.11	7.52
10	2	8	4.00	3.67	0.97	-3.54
10	3	1	2.91	2.85	2.21	-1.81
10	3	4	2.22	2.20	-2.02	0.88
10	4	0	3.48	3.63	-2.80	2.31
10	4	3	6.79	6.51	-5.12	4.03
11	0	2	4.78	4.79	0.57	4.76
11	1	1	5.35	5.73	-3.67	-4.39
11	1	4	1.78	1.70	1.46	1.03
11	1	7	6.36	5.70	2.16	5.28
11	2	0	11.59	10.88	-10.88	-0.48
11	2	3	6.82	6.72	0.66	-6.69
12	0	0	19.19	18.33	18.00	-3.47

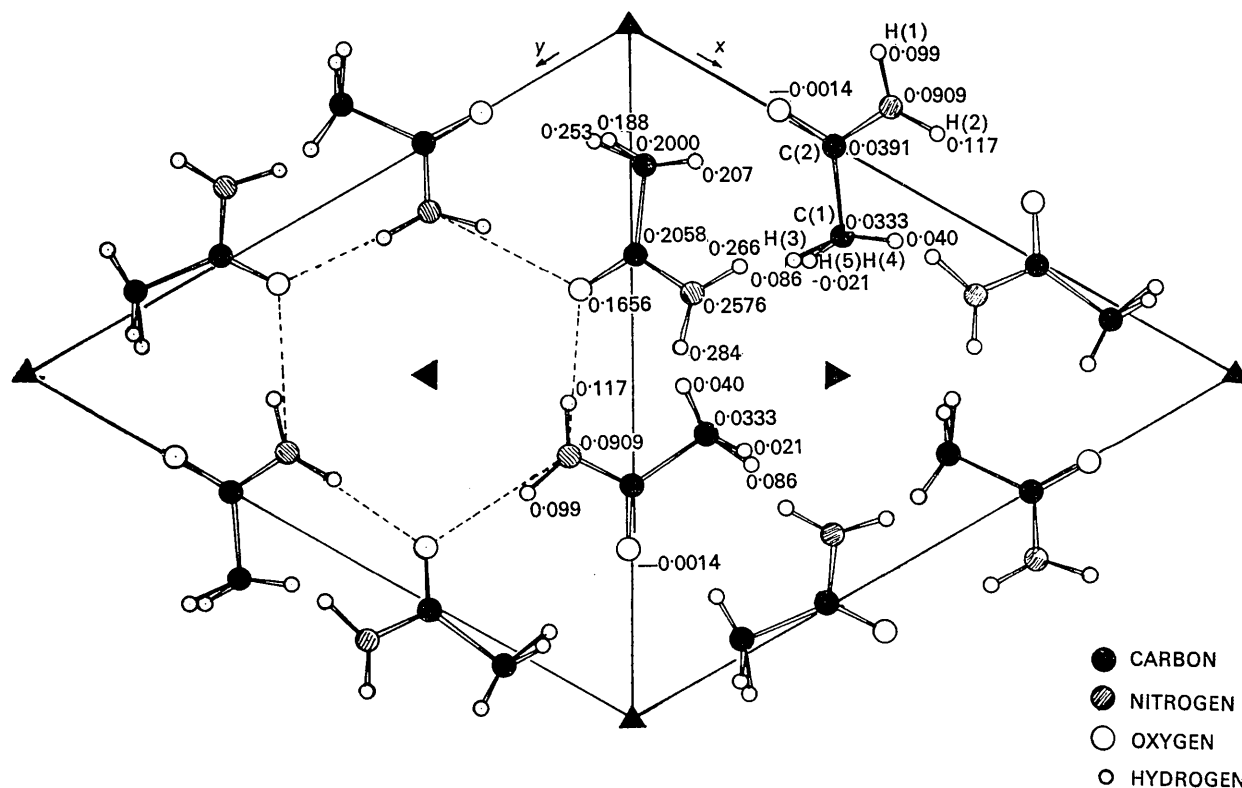
Fig. 1. Arrangement of one layer of molecules in rhombohedral acetamide. In addition to the threefold axes shown, there are 3_1 screw-axes passing approximately through each C(2) atom. Fractional z coordinates are shown.

roacetamide (Hughes & Small, 1962), difluoroacetamide (Hughes & Small, 1971) and trifluoroacetamide (Small, 1971) will be published later.

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