

Since the generation of a reciprocal lattice is a genuinely reciprocal process we could, as an equally valid alternative, have employed *selection* of points on the plane $x+y+z=0$ from a simple cubic lattice to represent D_{h_2} and would then have found that *projection* on this plane of the simple cubic reciprocal lattice reproduced R_{h_2} : the imaginary simple cubic lattices used for these two alternative representations have different orientations with respect to the direct hexagonal lattice.

Since selection of the points on one plane is equivalent to multiplication by a plane delta function, since the generation of a reciprocal lattice is equivalent to Fourier transformation, and since the Fourier transform of a plane delta-function is a rod delta-function normal to that plane, the whole representation (in either alternative) is an application of Parseval's theorem, namely that the Fourier transform of the operation 'multiply by' is 'fold with': folding a [111] rod delta-function with the simple cubic lattice points is equivalent, after discarding the superfluous dimension, to projection on the (111) plane.

Of the two alternative representations (the first, in which D_{h_2} is a projection, R_{h_2} a section, of a cubic lattice, and the second, in which D_{h_2} is a section, R_{h_2} a projection of a cubic lattice in another orientation) the first is to be preferred: it is only in this represen-

tation that names of points in D_{h_2} or R_{h_2} , according to customary conventions, correspond directly (save for scale factors) with their names in the cubic reference system. Now an inconsistency seems to have emerged, since in the earlier sections of this paper, while lattices were not under discussion, the re-lowering of dimensionality after introducing an auxiliary dimension was considered to be performed by taking a section. This was the effect of equation (2). However, the procedure in that part of the paper, which related to the descriptive crystallography of macroscopic bodies, clearly ought to correspond to the procedure employed for the representation of the direct, rather than that of the reciprocal lattice, namely a lowering of dimensionality by projection. The inconsistency is only apparent, since we also imposed equation (5); the projections and sections on plane (or hyperplane) (2) of all planes conforming to (5) are identical with each other. Projection for real space, section for reciprocal space is thus the representation applying consistently throughout.

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References

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The Crystal Structure of Orthorhombic Acetamide*

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The metastable form of acetamide has been studied by X-ray diffraction. The crystals are orthorhombic, space group *Pccn*, $a=7.76$, $b=19.00$, $c=9.51$ Å, $Z=16$. There are two molecules in the asymmetric unit. These are bound in two-molecule units by a pair of hydrogen bonds. Further hydrogen bonds link these dimers together in columns parallel to *c*. The average bond lengths in the planar molecules are C-C, 1.505 ± 0.013 ; C-N, 1.334 ± 0.017 ; C-O, 1.260 ± 0.011 , in good agreement with those in the stable (trigonal) solid phase, the vapor, and in similar compounds.

Introduction

Acetamide, $\text{CH}_3\text{CO-NH}_2$, exists in two crystalline modifications. The structure of the stable (trigonal) form has been reported by Senti & Harker (1940)†. The

metastable (orthorhombic) form at room temperature is obtained on cooling from the melt. The two forms differ markedly in their behavior when irradiated by γ rays (Rao, 1960). The principal products obtained from the irradiated crystals are acetonitrile (CH_3CN) and water. The yields per 100 eV of deposited energy are considerably greater for the trigonal form than for the orthorhombic. Since one would presume that the molecular structure is the same in both compounds, it must be details of the intermolecular interaction which are responsible for the differences in the radiation chemistry. In particular, one might expect the hydrogen bond-

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† A reinvestigation of this structure is presently being carried out by Mills, Harris & Harker (1964). The original investigation, carried out long before the age of the modern digital computer, is noteworthy for being the first example of the use of a Fourier refinement in an acentric structure.

ing to be considerably different in the two forms. This structure determination was undertaken with the hope of shedding some light on the chemical results.

Crystal data

Acetamide. Orthorhombic, *Pccn*. $a = 7.76 \pm 0.01$, $b = 19.00 \pm 0.04$, $c = 9.51 \pm 0.02$, $Z = 16$. X-ray density 1.119. The density of the trigonal form is 1.155.

Experimental

The crystals were prepared by cooling the melt slowly in Pyrex capillary tubes. Although there was occasional spontaneous reversion to the trigonal form, it was not difficult to select a few orthorhombic crystals for examination. The cell constants and space group were determined by Weissenberg and precession photography. The systematic absences ($0kl$, l odd; $h0l$, l odd; $hk0$, $h+k$ odd) indicate that the space group is probably *Pccn**. The reciprocal lattice nets $hk0$, $hk1$, \dots , $hk6$ were recorded with a Weissenberg camera and Cu $K\alpha$ radiation ($\lambda = 1.5418$). The intensities of 459 independent reflections were visually estimated and reduced to structure factors in the usual way by application of Lorentz and polarization corrections.

The solution of the structure was almost straightforward. A sharpened Patterson function with coefficients

$$F^2 \exp(8 \sin^2 \theta / \lambda^2) / \Sigma f_i^2$$

was calculated. From the Patterson function, $P(u, v, w)$, the *first order consistency function*:†

* Senti & Harker reported the space group as *Pbcn* for their orthorhombic crystals with similar cell constants.

† The use of *consistency functions* or *symmetry-adapted minimum functions* is implicit in Buerger's monograph (Buerger, 1959). This technique, called by Mighell & Jacobsen (1963) *vector verification*, has been briefly described by the author (Hamilton, 1963) and by Simpson & Lipscomb (1963) and has recently been given an especially elegant formulation by Ellison & Levy (1964). It has been used extensively by Kraut and coworkers for several years. (See, for example, Kraut, 1961). See also Simpson, Dobrott & Lipscomb (1965).

$$C_1(x, y, z) =$$

$$\text{Min} \{P(2x, 2y, 2z), \frac{1}{2}P(\frac{1}{2}, 2y, \frac{1}{2} + 2z), \frac{1}{2}P(2x, \frac{1}{2}, \frac{1}{2} + 2z), \frac{1}{2}P(\frac{1}{2} + 2x, \frac{1}{2} + 2y, 0), \frac{1}{4}P(\frac{1}{2} + 2x, 0, \frac{1}{2}), \frac{1}{4}P(0, \frac{1}{2} + 2y, \frac{1}{2}), \frac{1}{4}P(\frac{1}{2}, \frac{1}{2}, 2z)\}$$

was calculated to determine possible atomic positions (x, y, z) . The largest peak in the consistency function not near a symmetry element (where errors might possibly accumulate) was selected as the peak $(2x_0, 2y_0, 2z_0)$ corresponding to a possible atomic position (x_0, y_0, z_0) , and the following *second order consistency function* was calculated:

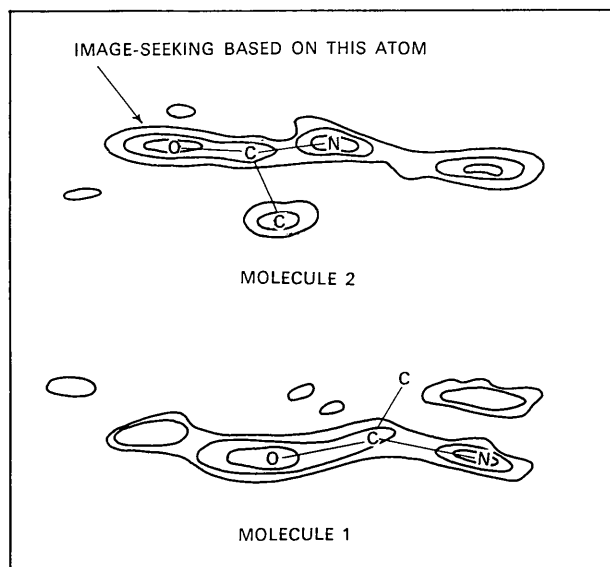


Fig. 1. Composite drawing of regions of the second order consistency function $C_2(x, y, z)$ in the neighborhood of the final coordinates of the two acetamide molecules in the asymmetric unit. The proper spatial relationships between the two molecules are not shown in the drawing. Although there were no other regions of $C_2(x, y, z)$ which showed peaks higher than the first contour in this drawing, the reader will note that there are spurious peaks in this region. In the initial stages of the structure refinement, the author was not fortunate enough to pick the correct peaks.

Table 1. Atomic parameters for orthorhombic acetamide

β_{ij} is defined so that the temperature factor may be written $\exp[-\sum_{i,j} \beta_{ij} h_i h_j]$. All parameters have been multiplied by 10^4 , and the estimated standard errors are in parentheses. Me indicates methyl.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{13}	β_{13}	β_{23}
Molecule 1									
C(1)	4890 (18)	7399 (7)	8578 (20)	145 (28)	36 (5)	167 (33)	- 1 (11)	+ 6 (28)	+ 13 (11)
Me(1)	5389 (21)	8150 (6)	8372 (18)	372 (42)	16 (4)	247 (35)	- 6 (10)	+ 14 (29)	+ 10 (8)
N(1)	4640 (15)	7022 (5)	7391 (14)	355 (33)	25 (4)	124 (24)	- 11 (9)	- 15 (22)	- 14 (7)
O(1)	4769 (15)	7144 (4)	9787 (14)	388 (30)	31 (3)	157 (23)	- 15 (8)	- 12 (21)	- 1 (6)
Molecule 2									
C(2)	2998 (19)	5340 (8)	9117 (21)	195 (31)	41 (6)	118 (33)	+ 14 (11)	+ 12 (28)	+ 24 (11)
Me(2)	2214 (19)	4612 (6)	9289 (17)	323 (38)	22 (4)	213 (29)	- 18 (10)	- 20 (28)	+ 13 (8)
N(2)	3165 (16)	5743 (6)	10235 (13)	339 (33)	30 (4)	105 (22)	- 8 (9)	- 4 (22)	- 4 (7)
O(2)	3496 (12)	5528 (4)	7901 (13)	294 (25)	34 (3)	132 (21)	- 13 (7)	- 7 (18)	- 3 (6)

$$C_2(x, y, z) =$$

$$\text{Min} \{P(x_0 - x, y_0 - y, z_0 - z), P(x_0 + x, y_0 + y, z_0 + z), \\ P(\frac{1}{2} - x + x_0, y + y_0, \frac{1}{2} + z + z_0), P(\frac{1}{2} + x + x_0, y_0 - y, \\ \frac{1}{2} + z_0 - z), P(x_0 + x, \frac{1}{2} + y_0 - y, \frac{1}{2} + z_0 + z), \\ P(x_0 - x, \frac{1}{2} + y_0 + y, \frac{1}{2} + z_0 - z), P(\frac{1}{2} + x_0 - x, \\ \frac{1}{2} + y_0 - y, z_0 + z), P(\frac{1}{2} + x_0 + x, \frac{1}{2} + y_0 + y, z_0 - z)\}.$$

If x_0, y_0, z_0 is the location of an atom in the crystal structure, then if an atom is also at x, y, z , $C_2(x, y, z)$ must be large. The function $C_2(x, y, z)$ revealed the broad outlines of the structure (Fig. 1); unfortunately, the distance between the centers of the two molecules in the asymmetric unit was in error by $\frac{1}{2}c$. After a few cycles of Fourier and least-squares refinements which failed to improve the agreement between observed and calculated structure factors to a satisfactory degree, the

error was recognized, and subsequent refinement by least squares led to the parameters in Table 1. The refinement was carried out on F with unit weights (which an error analysis showed was justified); the final value of the agreement factor was

$$R = \frac{\sum ||F_{\text{obs}}| - |F_{\text{calc}}||}{\sum |F_{\text{obs}}|} = 0.101.$$

The observed and calculated structure factors are presented in Table 2. The calculated values were obtained from the parameters in Table 1, scattering factors from *International Tables for X-ray Crystallography* (1962), and interlayer scale factors obtained by a refinement which included only isotropic temperature factors. The anisotropic temperature factors obtained in the final refinements may thus be expected to be

Table 2. Observed and calculated structure factors (in electrons) for acetamide

H	K	L	FOI	FCI	H	K	L	FOI	FCI	H	K	L	FOI	FCI	H	K	L	FOI	FCI	H	K	L	FOI	FCI	H	K	L	FOI	FCI	H	K	L	FOI	FCI		
...	L = 0	L = 2	L = 5	L = 6	L = 3	L = 4	L = 1		
0	0	432	432	3	2	16	16	1	0	61	61	3	12	8	8	4	7	6	6	4	2	12	11	0	18	5	3	3	17	5	5					
2	0	48	43	4	2	18	16	2	0	40	46	4	12	11	11	5	7	8	8	3	3	6	5	3	1	16	16	1	0	6	5					
4	0	50	48	5	2	4	5	3	0	25	22	0	13	9	8	2	8	18	19	4	3	6	5	5	3	13	12	4	1	5	5					
6	0	27	26	6	2	9	10	4	0	19	19	1	13	8	8	3	8	13	12	5	3	13	12	0	3	45	45	1	18	7	6					
1	1	45	48	1	3	6	6	1	1	4	4	2	13	6	6	5	8	12	10	0	4	10	3	1	3	25	21	...	L = 5	...	1	19	5	4		
3	1	30	23	2	3	4	1	2	1	51	53	3	13	4	3	4	7	6	5	2	3	13	13	...	L = 6	L = 6			
5	1	6	6	3	3	22	24	3	1	5	4	4	13	7	9	1	9	10	12	2	4	14	15	3	2	13	11	4	2	13	11	4	1	5	5	
7	1	8	10	4	4	32	28	4	1	19	19	0	14	13	13	2	9	12	13	3	4	9	9	4	2	5	4	0	2	5	4	0	2	19	23	
0	2	15	14	6	3	10	9	6	1	10	10	1	14	14	14	4	9	5	7	4	4	4	5	5	2	3	2	2	4	3	2	2	4	3	3	
2	2	182	196	1	4	12	9	0	2	45	34	2	14	10	11	1	10	19	16	0	5	33	29	2	2	3	2	2	4	3	2	2	4	3	3	
4	2	48	47	2	4	31	35	1	2	63	59	3	14	10	10	3	10	9	10	1	5	19	20	3	3	3	6	6	0	3	3	6	6	0	3	3
8	2	7	7	3	4	45	46	2	2	24	21	0	15	13	14	4	10	12	13	2	5	16	18	5	3	5	4	1	3	7	7	1	3	7	7	
1	3	64	63	4	4	43	44	3	2	14	14	1	15	13	13	5	10	13	12	4	5	5	6	1	4	32	30	2	3	6	8	8	2	3	6	8
3	3	17	17	6	4	5	4	4	2	19	17	2	15	7	10	1	12	4	5	2	7	4	3	3	5	14	13	4	4	5	10	11	4	4	4	
5	3	33	33	1	5	13	19	0	3	39	40	0	16	18	21	3	11	14	15	5	5	7	7	2	4	13	16	4	3	4	6	7	4	6	7	
0	4	153	132	2	5	17	25	2	3	31	33	1	16	10	9	1	11	5	6	1	6	26	23	4	4	7	8	1	4	7	8	1	4	7	6	
2	4	37	36	3	5	30	30	3	3	10	11	2	16	5	6	5	11	6	5	2	6	22	21	5	4	4	3	2	4	20	16	1	4	20	16	
4	4	35	31	4	5	17	18	4	3	27	26	4	16	6	6	6	11	4	4	4	6	9	8	6	4	6	7	0	5	5	1	5	4	1	5	4
6	4	10	10	6	5	9	10	4	4	8	7	1	17	10	10	1	12	4	5	2	7	4	3	0	7	19	20	2	5	10	8	1	5	4	4	
1	5	66	70	1	6	56	58	1	4	41	38	2	17	5	4	2	12	4	5	2	7	4	3	3	5	14	13	4	5	14	13	4	5	10	11	
3	5	26	26	2	6	43	44	2	4	4	3	1	4	17	4	6	3	12	18	19	3	7	14	13	1	6	28	31	5	5	4	4	4	4	4	
5	5	15	10	3	6	13	14	3	4	9	7	2	18	12	14	4	6	12	4	4	0	8	44	42	2	6	12	12	0	6	17	15	2	6	17	15
7	5	13	12	4	6	13	12	4	4	11	10	3	18	4	4	4	1	3	4	4	1	8	13	11	3	6	8	6	2	6	2	2	2	2	2	2
0	6	54	47	5	6	12	12	0	5	20	32	4	18	4	5	3	13	17	17	2	8	11	8	4	6	4	4	4	6	4	4	4	6	4	4	
2	6	24	9	6	6	12	13	1	5	16	11	1	19	6	5	4	13	7	6	4	8	5	5	5	6	6	6	0	7	7	11	10	7	9	7	
6	6	11	12	1	7	48	52	2	5	18	15	2	16	11	11	1	14	15	15	5	8	10	11	6	6	6	6	5	6	6	6	5	6	6	6	
1	7	6	11	2	7	28	30	3	5	5	6	...	L = 3	
5	7	20	18	4	7	8	8	5	5	4	5	...	L = 3	
0	8	114	104	5	7	15	14	6	5	12	12	1	1	14	12	1	15	9	11	2	9	6	6	4	7	7	8	1	8	6	5	1	8	6	5	
2	8	11	6	1	8	20	18	0	6	34	32	2	1	27	27	2	15	7	8	3	9	4	3	2	15	12	5	5	7	6	6	2	8	4	3	
6	8	8	4	3	8	35	35	1	6	3	4	3	1	11	12	3	11	12	3	3	11	12	3	6	5	4	9	6	6	3	8	3	3	3	3	
1	9	16	17	4	8	16	15	2	6	6	5	5	1	6	5	1	16	7	6	2	10	19	21	2	8	8	6	0	9	4	0	9	4	0	9	
3	9	10	7	1	9	27	26	3	6	17	16	6	1	4	4	2	16	8	9	3	10	13	14	3	8	14	14	1	9	5	4	1	9	5	4	
2	10	48	48	1	9	30	26	4	6	5	6	1	2	23	22	3	16	4	3	4	10	16	17	4	8	7	7	2	9	5	5	2	9	5	5	
4	10	14	11	2	10	10	18	5	6	5	5	3	2	5	4	5	17	6	5	4	10	20	22	5	8	5	5	3	9	7	8	8	8	8		
6	10	14	11	2	10	10	18	5	6	5	5	4	2	8	7	6	1	7	6	4	2	8	7	6	1	11	11	12	6	8	6	8	4	9	6	
1	11	19	18	4	9	11	10	1	7	27	26	1	3	52	51	4	17	6	5	3	11	12	12	3	9	15	16	3	9	15	16	3	9	15	16	
3	11	9	9	5	9	4	5	2	7	7	7	2	3	3	3	3	18	5	6	5	11	9	9	2	10	10	10	1	10	8	10	1	10	8	10	
5	11	10	11	1	10	29	26	3	7	3	2	3	3	11	11	4	18	5	6	0	12	19	18	3	10	10	10	2	10	8	9	2	10	8	9	
0	12	48	45	3	10	8	9	4	7	13	13	4	3	6	5	3	19	5	6	1	12	11	13	4	10	12	11	4	10	12	11	4	10	12	11	
4	12	6	6	5	10	9	5	7	4	4	3	5	3	6	6	6	3	20	3	4	2	12	27	28	2	11	7	7	2	11	7	7	2	11	7	
1	13	20	17	1	11	26	26	6	7	4	1	6	3	6	4	4	1	21	5	4	3	12	7	8	4	12	7	7	5	11	5	1	12	14	17	
3	13	16	16	2	11	12	12	0	8	21	16	1	4	5	4	1	4	12	7	7	5	11	5	1	12	14	17	5	11	5	1	12	14	17		
2	14	13	10	3	11	16	15	1	8	6	6	3	4	14	14	...	L = 4		
1	15	6	6	4	11	10	10	2	8	23	21	4	4	5	4	1	0	2	3	3	13	6	4	3	12	6	6	0	13	14	13	0	13	14	13	
5	15	12	12	1	12	17	17	3	8	9	10	5	4	5	6	6	4	14	13	4	13	7	8	4	12	7	7	0	14	7	9	0	14	7	9	
2	16	8	9	2	12	3	6	4	8	6	6	6	4	5	6	2	0	14	13	4	13	7	8	4	12	7	7	0	14	7	9	0	14	7	9	
3	17	9	11																																	

somewhat biased. A final difference electron density synthesis showed density in the regions where hydrogen atoms might be expected to lie. These positions were not refined, nor were hydrogen atom contributions included in the calculated structure factors.

The structure

The intramolecular interatomic distances are presented in Table 3. These are not unusual and are in satisfactory agreement with those found by Senti & Harker in the trigonal form, with the gas electron diffraction results of Kimura & Aoki (1953) and with similar bonds in urea (Worsham, Levy, & Peterson, 1957). Each of the molecules in the asymmetric unit is planar, and the deviations of the two molecules from a single plane, although significant, are not large. (See Table 4).

Table 4. *Least-squares planes* for acetamide with distances of atoms from planes*

Molecule 1	$7.503x - 4.841y - 0.155z + 0.036 = 0$
C(1)	-0.010 (0.014)
Me(1)	0.004 (0.016)
N(1)	0.003 (0.012)
O(1)	0.004 (0.011)
Molecule 2	$7.031x - 7.310y + 1.676z + 0.261 = 0$
C(2)	-0.007 (0.014)
Me(2)	0.002 (0.015)
O(2)	0.003 (0.012)
N(2)	0.002 (0.009)
Molecules 1 and 2	$7.266x - 6.433y + 0.885z + 0.290 = 0$
C(1)	-0.028 (0.014)
Me(1)	-0.166 (0.016)
N(1)	-0.072 (0.012)
O(1)	0.155 (0.011)
C(2)	-0.030 (0.014)
Me(2)	-0.117 (0.015)
N(2)	-0.069 (0.012)
O(2)	0.103 (0.009)

* Equations for the planes are in the form $Ax + By + Cz - D = 0$, where x , y , and z are fractional coordinates in terms of the unit translations, and $|D|$ is the distance of the plane from the origin in Å.

Intermolecular contacts less than 4.0 Å are presented in Table 5. These are normal. The four N...O distances less than 3.0 Å clearly correspond to the four crystallographically distinct hydrogen bonds in the structure; the hydrogen bonding will be discussed below.

The r.m.s. amplitudes of thermal motion along the principal axes of the vibrational ellipsoids are given in Table 6. The directions which the principal axes make with molecular axes were determined. Although these will not be cited here, it is worth noting that for each atom one of the principal axes is approximately perpendicular to the molecular plane. These axes are denoted by asterisks in the table. The shortest principal axis for each of the terminal atoms lies approximately along the bond to the central carbon. It would not seem particularly useful to carry out an analysis in terms of rigid body vibrations for such an extensively hydrogen-bonded system.

Table 5. *Intermolecular distances less than 4.0 Å*

An asterisk indicates a probable van der Waals contact. Column *A* contains distances between non-hydrogen-bonded molecules; column *H* contains distances between molecules which are linked by hydrogen bonds. The four short N-O distances are hydrogen bonds.

	<i>A</i>		<i>H</i>			
C-C	3.73*	3.76*				
C-Me	3.81*	3.96*				
C-N	3.67*	3.85	3.77	3.79	3.81	3.88
C-O		3.89	3.71	3.75	3.77	3.80
Me-Me	3.83*	3.98*				
Me-N	3.68*	3.90			3.88	
Me-O	3.57*	3.89			3.49*	
N-N	3.79	3.85			3.81	
N-O		3.96	2.87	2.94	2.97	3.01
O-O		3.77			3.69	

Table 6. *Root mean square amplitudes of vibration along principal axes of vibrational ellipsoid*

The components which lie closest to the normals to the molecular plane are indicated by an asterisk. For the terminal atoms, the shortest principal axis is always approximately along the bond to the central carbon atom.

	$\langle r_1^2 \rangle^{\ddagger}$	$\langle r_2^2 \rangle^{\ddagger}$	$\langle r_3^2 \rangle^{\ddagger}$
C(1)	0.19	0.23*	0.24
Me(1)	0.17	0.32	0.34*
N(1)	0.20	0.21	0.31*
O(1)	0.18	0.23	0.36*
C(2)	0.18*	0.23	0.26
Me(2)	0.19	0.28*	0.32
N(2)	0.21	0.23	0.27*
O(2)	0.21	0.25	0.28*

Hydrogen bonding

Two N-H...O hydrogen bonds connect the two independent molecules in the asymmetric unit into what might be called a dimer, were it not for the fact that these hydrogen bonds are slightly longer than those between the 'dimers'. Each molecule is hydrogen

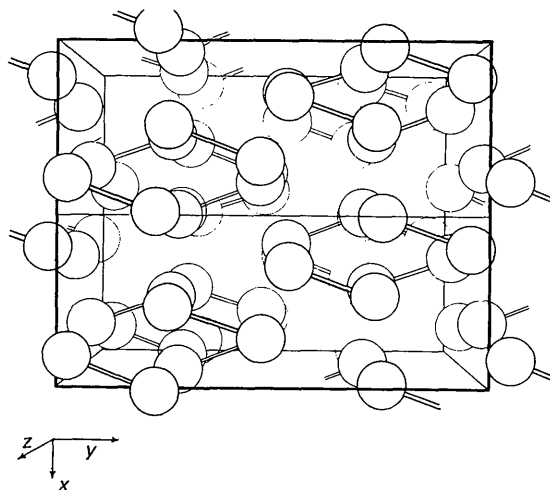


Fig. 2. The structure of orthorhombic acetamide viewed down the *c* axis. Two unit cells are shown. Each molecule is represented by a single circle. The double lines represent the two hydrogen bonds of the 'dimer'. The other hydrogen bonds link the molecules in chains approximately parallel to *c*. The four-strung columns are not linked to each other by hydrogen bonds.

Table 7. Distances (Å) and angles (°) associated with hydrogen bonds

A. In the 'dimer' (Between molecules 1 and 2)

O(1)-N(2)	2.971 (0.015)
N(1)-O(2)	3.014 (0.014)
O(1)-O(2)	3.691 (0.014)
N(1)-N(2)	3.813 (0.017)

Angle

C(1)-N(1)-O(2)	114.0 (1.0)
C(2)-N(2)-O(1)	116.5 (1.0)
C(1)-O(1)-N(2)	120.7 (1.0)
C(2)-O(2)-N(1)	120.1 (1.0)

B. Between molecule 1 at (X, Y, Z) and molecule 1' at (X, ½ - Y, -½ + Z)

N-O'	2.941 (0.016)
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Angle

C-N-O'	114.5 (0.9)
C'-O'-N	124.6 (0.9)

C. Between molecule 2 at (X, Y, Z) and molecule 2' at (½ - X, Y, ½ + z)

N-O'	2.873 (0.016)
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Angle

C-N-O'	125.9 (1.0)
C'-O'-N	135.0 (1.0)

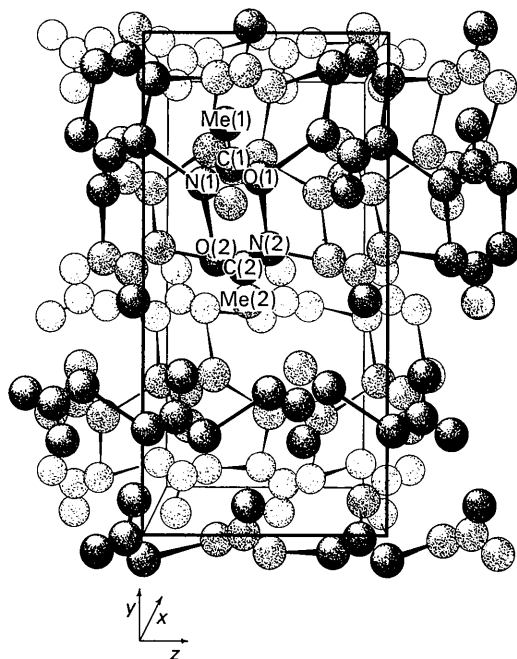


Fig. 3. The structure of orthorhombic acetamide viewed down the *a* axis, i.e. from the top of Fig. 2. All atoms except hydrogen are shown. The hydrogen bonds are indicated by heavy black lines. The atoms in one of the dimers are labeled (Me stands for methyl).

bonded to two of its own kind in chains parallel to the *c* axis. The result is a four-stringed column running through the lattice in the *c* direction. This is well-illustrated in Figs. 2 and 3. The hydrogen bonding is thus essentially one-dimensional in that if one were to wander through the lattice, always jumping from molecule to molecule along hydrogen bonds, he could travel as far as he liked in the *c* direction but would be limited to a few Ångströms of travel in the *a* and *b* directions. The hydrogen bonding in the trigonal form, on the other hand, consists of a beautiful three-dimensional network where every molecule in the crystal is connected to every other one through a continuous series of hydrogen bonds. Important distances and angles connected with the hydrogen bonding are presented in Table 7.

In view of the identical molecular structures in the two crystalline modifications of acetamide, it is clear that the very different hydrogen bonding scheme must play an important role in the radiation chemistry, but the exact mechanism is far from clear.

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