for the zones [010], [001], and [110] are 0·08, 0·10, and 0·12 if unobserved reflections are not considered. The detailed agreement is reasonable, and there can be little doubt of the essential correctness of the structure. The accuracy is less satisfactory, however. The mean standard deviation of light-atom coordinates has been estimated by Cruickshank's method (Lipson & Cochran, 1953) to be about 0·04 Å. This value is rather high, but perhaps not unduly so considering that the positions of these atoms have been derived from non-centrosymmetrical projections, and that there is an iron atom present.

Discussion

Intramolecular distances are given in Table 3. Individual deviations from mean distances in no case exceed the estimated standard deviation of light-atom coordinates, and are therefore not significant. The results agree well with those found by Ewens & Lister but can hardly be said to be more accurate.

Table 3. *Interatomic distances*

Atoms	Range (Å)	Mean (Å)	Standard deviation* (Å)	Value from Ewens & Lister (Å)
Fe, C	1·79 – 1·84	1·82	0·02	1·84 ± 0·03
C, O	1·11 – 1·15	1·14	0·02	1·15 ± 0·04
Fe, O	2·92 – 2·98	2·95	0·03	—

* Standard deviation from experimental values of equivalent distances. The standard deviation of light-atom coordinates, estimated by Cruickshank's method, is 0·04 Å.

The molecule has the form of a trigonal bipyramid, as expected, but if an idealized molecule is so oriented as to coincide as nearly as possible with the observed molecule, some distortion is evident. The displacement of any atom from its ideal position does not exceed 0·13 Å, but for three of the oxygen atoms, the displacements lie in the range 0·12 to 0·13 Å. These distances are about three times the estimated standard deviation of light-atom coordinates, and therefore represent a significant distortion. A consideration of intermolecular distances suggests a reason for the distortion. For the observed structure the shortest intermolecular distance is 3·03 Å, while for the idealized structure it is 2·89 Å. It would appear that the distortion of the molecule allows a closer packing, or in other words, that the molecule is sufficiently non-rigid to be deformed by van der Waals forces.

The specimens of iron pentacarbonyl were prepared by Dr K. F. H. Spiesecke of the Division of Pure Chemistry. The computations were carried out by Dr F. R. Ahmed of this laboratory, using IBM 650 computers at No. 1 Army Pay Ledger Unit, and at the University of Ottawa. Their assistance, and the continued encouragement of Dr W. H. Barnes, are gratefully acknowledged.

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The Crystal and Molecular Structure of Monofluoroacetamide

By D. O. Hughes and R. W. H. Small
Chemistry Department, University of Birmingham, England

(*Received* 13 *December* 1961)

The structure of monofluoroactamide has been determined using three-dimensional intensities measured with a proportional counter. Atomic positions and anisotropic thermal-vibration parameters have been refined by the least-squares method and the atomic thermal-vibration parameters interpreted in terms of the rigid-body vibrations of the molecule. The principal interatomic distances (corrected for rotational vibrations) are

$$\text{C–C} = 1{\cdot}533 \pm 0{\cdot}006,\ \text{C–F} = 1{\cdot}406 \pm 0{\cdot}005,\ \text{C–N} = 1{\cdot}319 \pm 0{\cdot}005,\ \text{C–O} = 1{\cdot}254 \pm 0{\cdot}005\ \text{Å}.$$

The determination of the structure of monofluoroacetamide forms part of a series of investigations being carried out in this laboratory to examine the influence of different attached groups and environments upon one particular group, the amide group. It is of interest also in respect of any effect the electronegative fluorine atom will have upon the hydrogen bonding system.

Unit cell data

Monofluoroacetamide has a melting point of 107 °C. and is volatile at room temperature. Suitable crystals were obtained by cooling a solution in ethyl alcohol; they were found to be triclinic showing the following forms, {010}, {001}, {012} and {101} with fairly even development. Cleavage parallel to (012) was noted.

Crystals were enclosed in Lindeman glass tubes for diffraction work; using Cu $K\alpha$ radiation the following cell dimensions were obtained from zero layer line Weissenberg photographs by the method of Bradley & Jay (1932) (assuming no absorption effects):

$$a=5\cdot103,\ b=5\cdot343,\ c=6\cdot901\ \text{Å}\ \ (\text{all } \pm 0\cdot005\ \text{Å})$$
$$\alpha=104^\circ\,46',\ \beta=100^\circ\,26',\ \gamma=100^\circ\,7'\ \ (\text{all } \pm 3')\,.$$

The convention of Buerger (1942) was adopted in choosing the unit cell. The density (1·45 g.cm.$^{-3}$, by flotation) indicated $Z_o=1\cdot97$.

Collection of intensity data

In the first instance, in order to establish the approximate structure only two-dimensional photographic data, visually estimated, were collected in the zones $0kl$, $h0l$, $hk0$. The statistical distribution of intensities in these zones revealed a centre of symmetry (Howells, Phillips & Rogers, 1950) indicating space group $P\bar{1}$, and the method of Wilson (1942) was used to obtain an absolute scale factor and an estimate of the temperature constant.

For refinement of the structure, three-dimensional data were collected using a proportional counter on the three-circle diffractometer (Small & Travers, 1961). The X-ray input to this instrument was monitored, the monitor counts being used as the basis for 'timing' the intensity measurements. To correct for drift in the electronic system and for the slow volatilisation of the crystal, a standard reflexion was measured after every ten intensity measurements. As a further safeguard after each new crystal was mounted a selection of previous measurements was checked for consistency. Crystals for measurement were coated with polystyrene so avoiding the uneven absorption effect which Lindeman tubes would introduce in this type of instrument. To avoid counting losses for strong reflexions and to differentiate weak ones from the background three sizes of crystal were used, approximately, 0·1, 0·2 and 0·4 mm. across. For most reflexions the middle size was suitable. Aluminium screens of predetermined absorption factor were used with the small crystals for the very strong reflexions, the crystals having been dipped in liquid air. Ten different crystals were used on account of the volatility and 600 of the 800 possible reflexions for Cu $K\alpha$ proved to be measurable.

As a consequence of the geometry of the three-circle diffractometer only Lorentz and polarization corrections have to be applied; the intensities were put on an approximately absolute scale by comparison with the photographic data.

Determination of the structure

Using the photographically estimated intensity data, sharpened Patterson projections on (100) and (010) were calculated. The function used to modify the coefficients was

$$M(S)=(1/\bar{f})^2 \exp\left(-\pi^2S^2/p\right)$$

where

$$S=2\sin\theta/\lambda \quad \text{and} \quad p=7\cdot25\,.$$

A ridge of peaks obtained in the projection on to (100) was interpreted as a series of parallel vectors of a molecule lying in the (012) plane. This was supported by the pronounced cleavage in this direction. The projection on (010) showed a number of distinct peaks, which could be explained by assuming probable bond lengths and bond angles and arranging the molecules as dimers, hydrogen-bonded about the origin with the carbon–carbon bond making an angle of approximately 35° with the c-axis. It was decided that the fluorine and nitrogen atoms would most probably occur on the same side of the molecule.

Projections of this trial structure on (010) and (001) were refined by Fourier, difference and least-squares methods. It was found necessary to assign individual isotropic temperature factors to the atoms at an early stage in the refinement. In the least-squares refinement weights of 0 and 1 were used and the off-diagonal terms were ignored. Two-dimensional refinement was discontinued when the discrepancy factors were $R_{h0l}=0\cdot18$ and $R_{hk0}=0\cdot16$. Difference Fourier series indicated that a large proportion of this residual was due to marked thermal anisotropy and that there was also a significant contribution from the hydrogen atoms.

Refinement of the three-dimensional data using the least squares programme (*SFLS*) of Dr J. S. Rollett was carried out on the MERCURY electronic computer at Oxford University. The initial weighting scheme chosen was

$$|F_o|>10,\ \ \sqrt{\omega}=10/|F_o|$$
$$|F_o|<10,\ \ \sqrt{\omega}=1$$

with only the atoms C_1, C_2, N, O, and F to compute the structure factors, four least-squares cycles reduced R to 0·125.

The positions of the hydrogen atoms were then obtained from a complete three-dimensional difference synthesis. The summation was carried out on the MERCURY computer using the three-dimensional Fourier programme of Mr O. S. Mills. The four highest maxima of electron density corresponded closely to the hydrogen positions expected for a trigonal arrangement about the nitrogen atom and a tetrahedral arrangement about the carbon atom. The hydrogen atoms were therefore assumed to be in these positions (Table 1) and were assigned the temperature factors of the atoms to which they were bonded. These positions and temperature factors were then used in the least-squares calculation of the structure factors. No attempt was made to refine the hydrogen parameters.

Table 1. *Atomic co-ordinates from three-dimensional difference synthesis*

	x/a	y/b	z/c
H_1	0·146	0·792	0·271
H_2	0·208	0·646	0·479
H_3	0·271	0·083	0·000
H_4	0·521	0·354	0·125

Four least squares cycles reduced R to 0·102. Investigations of the distribution of the residual between the observed and calculated structure amplitudes indicated that the weighting scheme needed to be modified to decrease the contribution from the weak reflections. Therefore using the weighting scheme

$$w = 1/[1 + (|F_o| - 4{\cdot}50/3{\cdot}50)^2]\,.$$

R was further reduced to 0·093.

The average co-ordinate shift at the end of the last least-squares cycle was 0·00008 Å and the largest 0·00015 Å. The final co-ordinates are shown in Table 2. This represented the limit of least squares refinement and a final three-dimensional difference synthesis revealed no significant features that might have been overlooked. Table 10 shows final values of the observed and calculated structure factors.

Table 2. *Atomic co-ordinates from final least-squares cycle*

	x/a	y/b	z/c
C_1	0·26585	0·66657	0·34212
C_2	0·15627	0·38743	0·19472
N	0·32744	0·26388	0·11345
O	0·90700	0·28981	0·16024
F	0·54641	0·74415	0·36622

Analysis of the anisotropic thermal motion

In the course of the least squares refinement the atomic scattering factors were modified by a temperature factor of the form

$$2^{-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + b_{12}hk + b_{23}kl + b_{13}hl)}$$

depending on six parameters b_{ij} different for each atom, the values shown in Table 3 are from the final least-squares cycle.

If the thermal motion of an atom is considered in terms of an ellipsoid of vibration the temperature constants b_{ij} can be related to the constants of this ellipsoid (Rollett & Davies, 1955). Thus using a programme of Dr R. Sparks it was possible to compute the magnitudes of the principal axes of each ellipsoid and the direction cosines relative to three orthogonal axes a, b', c^* from the final values of b_{ij}.

Molecular axes L, M, N were chosen where L was parallel to the carbon–carbon bond, M was perpendicular to L in the plane of the amide group and N was perpendicular to L and M. The origin was taken at the centre of mass. The mean square amplitudes of vibration of each atom in the directions, L, M and N were then calculated. The values (Å²) obtained are given in Table 4.

Table 4. *Mean square amplitudes of vibration*

	r^2_L	r^2_M	r^2_N
C_1	0·0315	0·0484	0·0647
C_2	0·0339	0·0381	0·0389
N	0·0322	0·0409	0·0609
O	0·0382	0·0359	0·0817
F	0·0298	0·0479	0·1152

If the phase independence of the various molecular vibrations is assumed, the formula of Higgs (1955),

$$\bar{u}_x^2 = \Sigma(\bar{u}_x^2)\ \text{(rigid body)} + \Sigma(\bar{u}_x^2)\ \text{(internal)}$$

can be used to obtain a series of equations which express the observed mean-square amplitudes as the sum of rigid-body translation vibrations along L, M, N, rigid-body libration vibrations about these axes, and independent atomic vibrations. To obtain any solution the number of unknowns must be kept to a minimum and so it was necessary to postulate some simple model. The model chosen was a molecule vibrating as a rigid body, with an extra mode of vibration due to twisting of the fluorine atom about the carbon–carbon bond. In addition it was necessary to consider that the molecules are not vibrating as individual entities but as part of a complex hydrogen-bonded arrangement. In consequence there will be a certain restoring force, the apparent effect of which will be to shift the centre of mass an amount δL along the L-axis towards the amide group.

Table 3. *Anisotropic thermal vibration parameters b_{ij}*

	b_{11}	b_{22}	b_{33}	b_{23}	b_{31}	b_{12}
C_1	0·03628	0·03256	0·02224	−0·00279	0·00653	0·00211
C_2	0·02829	0·02859	0·01762	0·01128	0·00439	0·00539
N	0·03060	0·03098	0·02253	0·00101	0·00639	0·00283
O	0·02730	0·03678	0·03042	−0·00124	0·00944	0·00471
F	0·04050	0·04257	0·03690	−0·01684	0·01668	−0·02999

On the basis of this model, motion parallel to each of the three axes (L, M, N) was considered in turn, the values obtained for the mean square amplitudes of rigid-body translation (t^2_L, t^2_M, t^2_N, Å^2) and the mean square amplitudes of rigid-body libration (ω^2_L, ω^2_M, ω^2_N, radian^2) are given in Table 5.

Table 5. *Vibration amplitudes*

t^2_L	0·030	ω^2_L	0·0163
t^2_M	0·037	ω^2_M	0·0175
t^2_N	0·036	ω^2_N	0·0042

The value obtained for the shift of the centre of oscillation away from the centre of mass (δL) was 0·247 Å and the mean square amplitude of twisting of the bond C_1–F about the C_1–C bond (L axis) was 0·0127 radian^2.

Cruickshank (1956, 1961) has demonstrated that in high-accuracy structure determinations there is a significant error introduced in atomic positions due to rotational oscillation. The approximate corrections (ΔL, ΔM, ΔN) to be applied to the atomic co-ordinates L, M, N (referred to the molecular axes, with the centre of oscillation as origin) can be obtained from the relations

$$-\Delta L = \tfrac{1}{2}L\,(\omega^2_M+\omega^2_N)$$
$$-\Delta M = \tfrac{1}{2}M(\omega^2_L+\omega^2_N)$$
$$-\Delta N = \tfrac{1}{2}N\,(\omega^2_L+\omega^2_M)$$

Using the above expressions it was thus possible to calculate the corrections necessary to apply to the bond lengths.

Results

The values obtained for the bond lengths and bond angles are shown in Fig. 1 and Table 6. The arrangement of the molecules is shown in Fig. 2.

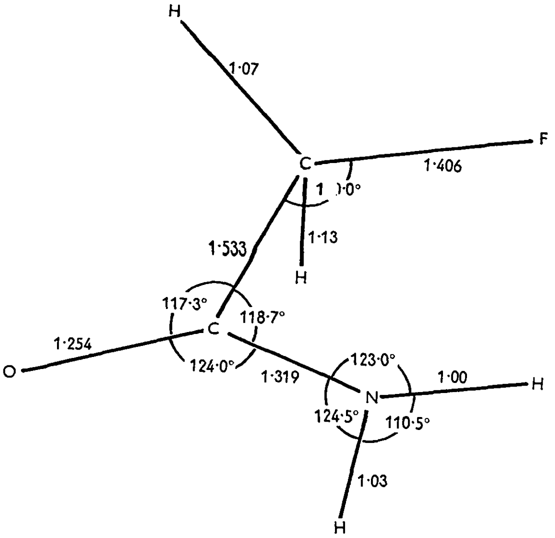

Fig. 1. Bond lengths and bond angles.

The standard deviations of the co-ordinates of the atoms C_1, C_2, N, O and F were estimated from the final least-squares cycle (*International Tables for X-ray Crystallography*, 1959). The values obtained are shown in Table 7 and the resultant standard deviations in bond lengths and bond angles are shown in Table 8.

Table 6. *Bond lengths and bond angles*

Bond	Uncorrected length	Corrected length
C_1–C_2	1·516 Å	1·533 Å
C_1–F	1·385	1·406
C_2–N	1·306	1·319
C_2–O	1·241	1·254
C_1–H_1	1·13	—
C_1–H_2	1·07	—
N–H_3	1·03	—
N–H_4	1·00	—
Angle	Uncorrected	Corrected
C_2–C_1–F	110° 00′	109° 59′
C_1–C_2–O	117° 17′	117° 16′
C_1–C_2–N	118° 41′	118° 42′
O–C_2–N	124° 2′	124° 2′
C_2–C_1–H_1	104° 27′	—
C_2–C_1–H_2	102° 27′	—
H_1–C_1–H_2	111° 10′	—
Angle	Uncorrected	Corrected
F–C_1–H_1	114° 3′	—
F–C_1–H_2	115° 6′	—
C_2–N–H_3	124° 33′	—
C_2–N–H_4	122° 57′	—
H_3–N–H_4	110° 32′	—

Table 7. *Standard deviations in co-ordinates* (Å)

	x	y	z
C_1	0·0041	0·0043	0·0045
C_2	0·0036	0·0040	0·0039
N	0·0032	0·0035	0·0036
O	0·0026	0·0031	0·0033
F	0·0027	0·0029	0·0032

Table 8. *Standard deviations in bond-lengths and bond-angles*

Bond	σ (Å)	Angle	(σ°)
C_1–C_2	0·006	C_2–C_1–F	0·4
C_1–F	0·005	C_1–C_2–O	0·4
C_2–O	0·005	C_1–C_2–N	0·4
C_2–N	0·005	O–C_2–N	0·4

The standard deviations of hydrogen co-ordinates were obtained from the earlier three-dimensional difference synthesis, using the method of Cruickshank (1949). The standard deviation of any hydrogen co-ordinate was estimated as 0·03 Å, giving a standard deviation of bond length of 0·05 Å for the bonds to hydrogen atoms and a standard deviation of 5° for angles involving such bonds.

The atoms C_1, C_2, N, O, and F are coplanar within the limits of experimental error, the equation of the plane being

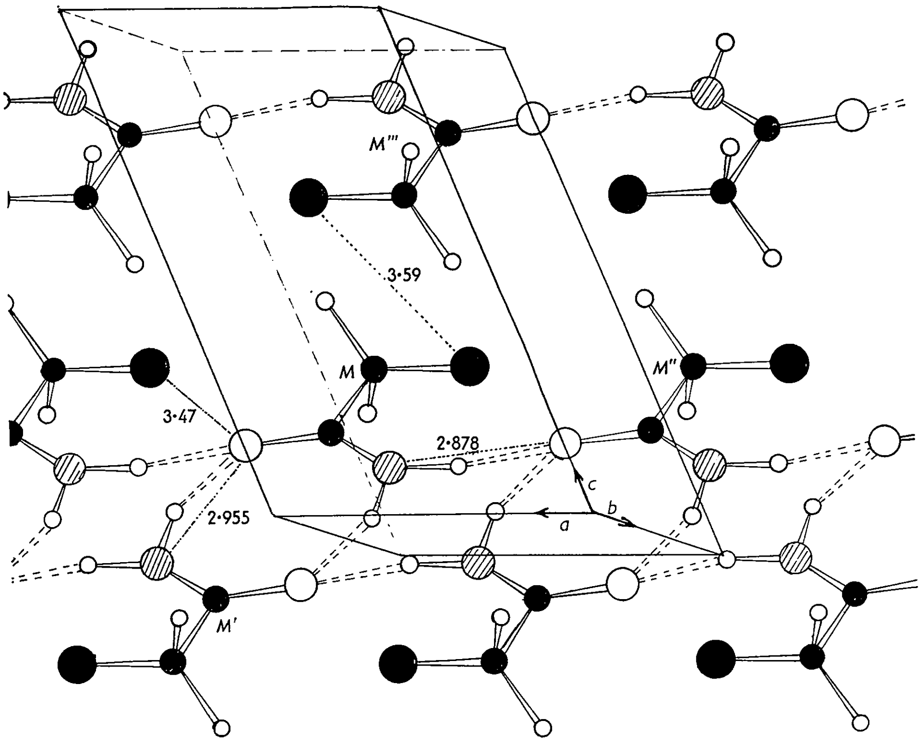

Fig. 2. Arrangement of the molecules.

$$0\cdot0896x-0\cdot63602y+0\cdot76643z+0\cdot05951=0$$

referred to the orthogonal axes a, b', c^*. The values of the coefficients were determined by the method of least squares. The perpendicular displacements of individual atoms from this plane are shown in Table 9.

Table 9. *Displacement from mean plane of molecule*

Atom	(Å)	Atom	(Å)
C_1	−0·006	H_3	−0·10
C_2	−0·003	H_4	−0·15
N	0·001	O′	0·113
O	0·006	O″	0·464
F	0·004		

The crystal structure

Molecules are arranged in layers almost parallel to $(01\bar{2})$ (Fig. 2). Each layer is made up of parallel ribbons of hydrogen-bonded molecules, the extension of the ribbons being in the direction of the a axis. The ribbons consist of pairs of molecules hydrogen bonded about a centre of symmetry with further hydrogen bonds to molecules related by the a-translation. Each oxygen and nitrogen forms two hydrogen bonds thereby making use of both amide hydrogen atoms.

As the distances in Table 9 indicate, the molecules forming the hydrogen-bonded layers are not exactly coplanar, the angle of tilt between the molecular planes and the N · · · O bond directions (between neighbours related by the a translation) being about 5°; this is larger than the tilt of 2° found in formamide and 1° in oxamide and succinamide. Repulsion between the fluorine atoms in molecules M and M''' may account for the greater tilt found in this structure.

The hydrogen bonds linking the centro-symmetrically related molecules M and M' are of length (N · · · O) 2·955 Å with the hydrogen atom 1·03 Å from the nitrogen and 1·97 Å from the oxygen, the N–H bond making an angle of 11° to the N · · · O direction. The bonds between molecules M and M'' are 2·878 Å (N · · · O) the N–H and O–H distances respectively being 1·00 Å and 2·03 Å, in this case the N–H bond makes an angle of 26° to the direction N · · · O. The fluorine atoms do not take part in the intermolecular hydrogen bonding system, the nearest approach being to an oxygen atom (3·47 Å).

The thermal vibrations of the molecule are clearly influenced by the hydrogen bonds. The translational components of the thermal motion are fairly isotropic (Table 5), the mean square amplitude of angular vibration about the axis N (which is perpendicular to the molecular plane and the hydrogen-bonding system) being only one quarter of that about the axes L and M which produce out-of-plane vibration (Table 5). The field due to the hydrogen bonding has a marked restraining affect on the angular vibration at the amide end of the molecule as shown by the shift of 0·247 Å of the centre of rotation from the centre of mass towards the amide group.

Table 10. *Observed and calculated structure factors*

h k ℓ	F_o	F_c
0 0 1	4.96	5.22
0 0 2	13.14	-13.10
0 0 3	3.74	-4.06
0 0 4	13.24	-13.50
0 0 5	1.22	1.62
0 0 6	3.92	3.98
0 0 7	1.28	-1.40
0 1 0	15.58	-17.72
0 1 1	5.58	-5.62
0 1 2	28.84	-29.66
0 1 3	3.74	3.74
0 1 4	9.06	9.08
0 1 5	1.62	-1.68
0 1 $\bar{1}$	4.88	5.04
0 1 $\bar{2}$	44.32	48.68
0 1 $\bar{3}$	4.10	4.40
0 1 $\bar{4}$	6.26	-5.88
0 1 $\bar{5}$	1.62	-1.76
0 1 $\bar{6}$	4.10	-4.58
0 1 $\bar{7}$	0.80	0.92
0 1 $\bar{8}$	1.06	1.36
0 2 0	28.92	-30.74
0 2 1	5.84	5.44
0 2 2	15.06	14.18
0 2 3	1.90	-1.66
0 2 4	3.92	4.00
0 2 7	0.60	0.52
0 2 $\bar{1}$	7.84	-7.46
0 2 $\bar{2}$	10.18	-10.34
0 2 $\bar{3}$	3.40	3.14
0 2 $\bar{4}$	17.06	17.16
0 2 $\bar{5}$	1.42	1.58
0 2 $\bar{6}$	1.90	-2.12
0 2 $\bar{8}$	0.98	-1.26
0 3 0	12.72	12.36
0 3 1	0.94	-0.64
0 3 2	6.88	6.42
0 3 4	2.78	-2.62
0 3 6	0.76	-0.98
0 3 $\bar{1}$	2.70	2.80
0 3 $\bar{2}$	15.24	-14.70
0 3 $\bar{3}$	5.14	-5.12
0 3 $\bar{4}$	4.36	-4.50
0 3 $\bar{5}$	1.20	1.26
0 3 $\bar{6}$	5.22	5.70
0 4 0	4.44	4.40
0 4 2	3.40	-3.26
0 4 4	1.90	-1.92
0 4 5	0.96	-1.18
0 4 $\bar{1}$	1.02	0.86
0 4 $\bar{2}$	6.54	6.50
0 4 $\bar{3}$	0.84	1.14
0 4 $\bar{4}$	4.36	-4.90
0 4 $\bar{5}$	2.00	-2.28
0 4 $\bar{6}$	2.08	-2.18
0 4 $\bar{8}$	1.28	1.86
0 5 0	2.00	-2.12
0 5 2	2.08	-2.22
0 5 3	0.70	-0.82
0 5 $\bar{2}$	1.02	1.32
0 5 $\bar{4}$	2.36	2.98
0 5 $\bar{6}$	0.90	-1.26
0 6 0	1.00	-1.52
0 6 1	0.52	-0.62
0 6 $\bar{5}$	0.60	0.16
0 6 $\bar{6}$	0.44	1.26
1 0 0	4.96	-5.06
1 0 2	8.62	-7.92
1 0 3	13.76	-12.58
1 0 4	2.00	2.28
1 0 5	2.50	2.96
1 0 6	1.24	1.22
1 0 $\bar{1}$	22.56	25.94
1 0 $\bar{2}$	3.14	-3.84
1 0 $\bar{3}$	12.28	-12.98
1 0 $\bar{4}$	8.18	8.02
1 0 $\bar{5}$	1.46	0.98
1 0 $\bar{6}$	2.00	1.64
1 0 $\bar{7}$	0.98	1.08
1 0 $\bar{8}$	3.30	-3.06
1 1 0	6.96	-6.30
1 1 1	17.60	-17.00
1 1 2	4.88	4.52
1 1 3	2.62	2.76
1 1 4	2.70	2.88
1 1 5	1.36	1.56
1 1 $\bar{2}$	6.26	-6.08
1 1 $\bar{3}$	11.14	9.46
1 1 $\bar{4}$	1.70	-2.14
1 1 $\bar{5}$	5.22	-4.96
1 1 $\bar{6}$	3.40	3.00
1 1 $\bar{7}$	0.76	0.76
1 1 $\bar{8}$	1.14	1.24
1 $\bar{1}$ 0	2.70	-2.16
1 $\bar{1}$ 1	25.60	28.98
1 $\bar{1}$ 4	5.74	-5.30
1 $\bar{1}$ 5	5.66	-5.94
1 $\bar{1}$ 7	2.08	2.18
$\bar{1}$ 1 1	18.02	-18.14
$\bar{1}$ 1 2	13.58	12.52
$\bar{1}$ 1 4	2.44	2.12
$\bar{1}$ 1 5	4.10	3.90
$\bar{1}$ 1 6	6.54	-6.46
$\bar{1}$ 1 7	2.00	-1.76
$\bar{1}$ 1 8	0.96	1.18
1 2 0	5.32	5.02
1 2 1	2.52	1.86
1 2 3	3.22	3.16
1 2 4	0.88	-0.88
1 2 6	1.48	-1.84
1 2 $\bar{1}$	11.24	-9.92
1 2 $\bar{2}$	5.14	-4.44
1 2 $\bar{3}$	0.70	0.92
1 2 $\bar{4}$	2.52	-2.66
1 2 $\bar{5}$	2.88	2.82
1 2 $\bar{6}$	1.30	-1.38
1 2 $\bar{8}$	0.74	0.72
1 $\bar{2}$ 0	10.72	9.02
1 $\bar{2}$ 1	14.20	-15.58
1 $\bar{2}$ 2	2.18	2.42
1 $\bar{2}$ 3	15.24	15.34
1 $\bar{2}$ 4	1.78	1.50
1 $\bar{2}$ 6	2.44	-2.38
$\bar{1}$ 2 1	4.78	-4.78
$\bar{1}$ 2 2	3.40	3.54
$\bar{1}$ 2 3	7.76	7.58
$\bar{1}$ 2 4	10.28	-10.26
$\bar{1}$ 2 5	2.88	-2.68
$\bar{1}$ 2 6	2.62	2.54
$\bar{1}$ 2 7	0.62	0.50
1 3 0	2.62	2.54
1 3 1	2.44	2.42
1 3 2	1.68	-1.52
1 3 3	0.92	1.00
1 3 4	2.96	-2.98
1 3 5	1.60	-1.88
1 3 $\bar{2}$	4.36	3.88
1 3 $\bar{3}$	2.18	-2.48
1 3 $\bar{4}$	1.64	-1.76
1 3 $\bar{5}$	1.22	-1.02
1 3 7	1.12	1.04
1 $\bar{3}$ 0	2.52	2.52
1 $\bar{3}$ 1	4.62	-4.44
1 $\bar{3}$ 2	2.08	1.88
1 $\bar{3}$ 3	7.40	-7.44
1 $\bar{3}$ 4	1.20	1.42
1 $\bar{3}$ 5	6.44	6.80
1 $\bar{3}$ 6	1.34	1.22
1 $\bar{3}$ 7	0.90	-1.04
1 $\bar{3}$ 8	0.48	-1.08
$\bar{1}$ 3 1	9.32	9.16
$\bar{1}$ 3 2	9.76	10.90
$\bar{1}$ 3 3	2.70	-2.66
$\bar{1}$ 3 4	3.48	3.64
$\bar{1}$ 3 6	3.48	3.14
1 4 0	1.28	-1.50
1 4 1	1.76	1.78
1 4 2	3.04	-3.12
1 4 3	2.26	-2.28
1 4 $\bar{2}$	1.24	1.14
1 4 $\bar{3}$	0.92	0.72
1 4 $\bar{4}$	1.66	2.02
1 $\bar{4}$ 0	7.48	-6.96
1 $\bar{4}$ 1	6.80	6.64
1 $\bar{4}$ 2	0.98	1.18
1 $\bar{4}$ 3	2.08	-2.48
1 $\bar{4}$ 4	0.72	-0.70
1 $\bar{4}$ 5	2.44	-2.80
1 $\bar{4}$ 7	2.26	2.76
$\bar{1}$ 4 1	2.00	-1.94
$\bar{1}$ 4 2	3.14	3.44
$\bar{1}$ 4 4	4.10	3.92
$\bar{1}$ 4 5	0.72	0.76
1 5 0	1.96	-2.16
1 5 1	1.48	-1.86
1 5 $\bar{1}$	1.68	1.78
1 5 $\bar{3}$	1.48	-1.52
1 5 $\bar{5}$	1.24	1.12
1 $\bar{5}$ 0	2.44	2.52
1 $\bar{5}$ 1	1.48	-1.30
1 $\bar{5}$ 2	2.96	-2.90
1 $\bar{5}$ 3	3.14	3.04
1 $\bar{5}$ 4	0.68	0.80
1 $\bar{5}$ 6	0.68	-0.81
1 $\bar{5}$ 7	0.62	-1.14
$\bar{1}$ 5 2	3.30	3.22
$\bar{1}$ 5 3	0.44	0.60
1 6 0	0.34	0.26
1 $\bar{6}$ 0	1.82	1.62
1 $\bar{6}$ 2	1.54	1.36
1 $\bar{6}$ 3	0.88	-0.72
1 $\bar{6}$ 4	1.00	-1.02
2 0 0	0.96	-1.08
2 0 1	1.58	-1.88
2 0 2	11.40	10.42
2 0 3	4.18	3.90
2 0 6	3.48	3.16
2 0 $\bar{1}$	7.06	-6.58
2 0 $\bar{2}$	12.02	-13.92
2 0 $\bar{3}$	3.66	-3.68
2 0 $\bar{4}$	2.70	-2.44
2 0 $\bar{5}$	5.06	4.50
2 0 $\bar{6}$	3.92	3.54
2 0 $\bar{7}$	1.70	1.44
2 1 0	15.42	17.40
2 1 1	5.58	5.08
2 1 2	2.88	-2.42
2 1 4	6.88	-6.52
2 1 6	1.36	1.76
2 1 $\bar{1}$	2.00	-2.44
2 1 $\bar{2}$	0.52	-0.56
2 1 $\bar{3}$	4.70	-4.48
2 1 $\bar{4}$	6.62	-6.22
2 1 $\bar{5}$	2.62	-2.18
2 1 $\bar{6}$	1.04	-1.00
2 1 $\bar{7}$	1.58	1.24
2 1 $\bar{8}$	1.22	1.32
2 $\bar{1}$ 0	13.68	-13.54
2 $\bar{1}$ 1	7.14	-6.74
2 $\bar{1}$ 2	0.34	-0.36
2 $\bar{1}$ 3	1.38	-1.04
2 $\bar{1}$ 4	3.48	3.32
2 $\bar{1}$ 5	1.48	1.88
2 $\bar{1}$ 6	1.54	1.46
$\bar{2}$ 1 1	4.18	-5.70
$\bar{2}$ 1 2	3.14	-3.90
$\bar{2}$ 1 3	8.54	9.34
$\bar{2}$ 1 4	7.76	8.10
$\bar{2}$ 1 5	1.18	1.08
$\bar{2}$ 1 7	3.66	-3.64
$\bar{2}$ 1 8	1.02	-1.20
2 2 0	3.92	3.16
2 2 1	0.64	0.60
2 2 2	11.58	10.98
2 2 3	1.18	-1.40
2 2 4	3.48	4.36
2 2 $\bar{1}$	5.66	5.50
2 2 $\bar{2}$	16.38	13.14
2 2 $\bar{3}$	1.04	-1.14
2 2 $\bar{4}$	1.08	-0.94
2 2 $\bar{5}$	0.98	-1.00
2 2 $\bar{6}$	1.60	-1.68
2 2 $\bar{7}$	1.84	-1.30
2 2 $\bar{8}$	0.60	-0.52
2 $\bar{2}$ 0	4.78	-4.22
2 $\bar{2}$ 1	4.44	-4.54
2 $\bar{2}$ 2	5.06	-4.84
2 $\bar{2}$ 3	2.96	-3.16
2 $\bar{2}$ 4	1.34	-1.18
2 $\bar{2}$ 5	0.82	-0.80
2 $\bar{2}$ 6	0.60	0.54
2 $\bar{2}$ 7	0.42	0.82
$\bar{2}$ 2 1	10.54	11.74
$\bar{2}$ 2 2	10.98	12.20
$\bar{2}$ 2 3	0.54	0.66
$\bar{2}$ 2 4	0.82	-0.62
$\bar{2}$ 2 5	6.54	-6.90
$\bar{2}$ 2 6	2.78	-2.70
$\bar{2}$ 2 7	1.70	1.54
2 3 0	12.62	-11.96
2 3 1	1.40	-1.64
2 3 2	6.88	6.60
2 3 $\bar{2}$	1.60	-1.56
2 3 $\bar{3}$	3.66	3.82
2 3 $\bar{4}$	6.26	6.04
2 3 $\bar{6}$	1.10	-0.98
2 $\bar{3}$ 0	10.54	9.46
2 $\bar{3}$ 1	9.58	8.86
2 $\bar{3}$ 2	3.30	-2.90
2 $\bar{3}$ 3	2.18	-2.20
2 $\bar{3}$ 6	1.40	-1.30
$\bar{2}$ 3 1	0.82	0.98
$\bar{2}$ 3 2	0.88	-1.06
$\bar{2}$ 3 3	8.18	9.46
$\bar{2}$ 3 4	4.62	-4.66
$\bar{2}$ 3 5	3.14	3.16
$\bar{2}$ 3 6	0.98	0.88
2 4 0	6.80	6.34
2 4 2	3.40	3.06
2 4 $\bar{2}$	8.54	-8.22
2 4 $\bar{3}$	0.72	-0.66
2 4 $\bar{4}$	1.20	0.18
2 4 $\bar{5}$	1.32	1.66
2 4 $\bar{6}$	2.02	2.12
2 $\bar{4}$ 1	1.02	1.24
2 $\bar{4}$ 2	4.88	4.36
2 $\bar{4}$ 3	3.22	3.66
2 $\bar{4}$ 4	1.06	-1.26
2 $\bar{4}$ 5	0.96	-0.90
2 $\bar{4}$ 6	0.76	0.96
$\bar{2}$ 4 1	8.96	-9.26
$\bar{2}$ 4 2	4.70	-5.08
$\bar{2}$ 4 3	4.18	4.10
$\bar{2}$ 4 4	1.82	1.60
$\bar{2}$ 4 5	2.70	2.36
2 5 0	3.04	2.82
2 5 $\bar{2}$	3.80	3.96
2 5 $\bar{3}$	0.84	-1.10
2 5 $\bar{4}$	3.30	-4.30
2 5 $\bar{5}$	0.74	-0.60
2 5 $\bar{6}$	0.60	0.52
2 $\bar{5}$ 0	4.10	-3.54
2 $\bar{5}$ 1	6.80	-6.20
2 $\bar{5}$ 3	1.02	1.16
2 $\bar{5}$ 4	1.58	1.48
2 $\bar{5}$ 5	0.92	0.92
$\bar{2}$ 5 1	3.58	3.52
$\bar{2}$ 5 2	1.96	1.96
$\bar{2}$ 5 3	2.88	2.76
$\bar{2}$ 5 4	0.96	1.00
2 $\bar{6}$ 0	1.76	1.66
2 $\bar{6}$ 1	2.18	2.14
2 $\bar{6}$ 2	1.62	-1.84
2 $\bar{6}$ 3	2.88	-3.00
$\bar{2}$ 6 1	2.52	2.36
3 0 0	4.36	-4.00
3 0 1	14.62	13.52
3 0 2	1.62	1.52
3 0 3	3.48	3.00
3 0 4	0.82	-0.88
3 0 5	6.36	-6.30
3 0 6	0.54	-0.82
3 0 $\bar{1}$	7.14	-7.68
3 0 $\bar{2}$	6.44	6.50
3 0 $\bar{3}$	4.36	-4.04
3 0 $\bar{4}$	1.44	-1.10
3 0 $\bar{6}$	2.18	-2.16
3 0 $\bar{8}$	1.26	1.32
3 1 1	4.00	3.86
3 1 3	12.02	-11.22
3 1 4	0.82	-0.96
3 1 5	2.08	2.34
3 1 $\bar{1}$	13.42	13.72
3 1 $\bar{2}$	5.22	-4.04
3 1 $\bar{3}$	5.58	-5.22
3 1 $\bar{4}$	5.84	5.40
3 1 $\bar{5}$	0.60	-0.74
3 1 $\bar{8}$	1.02	-1.12
3 $\bar{1}$ 0	4.00	4.04
3 $\bar{1}$ 2	1.62	-1.30
3 $\bar{1}$ 3	7.32	7.26
3 $\bar{1}$ 4	1.86	1.66
3 $\bar{1}$ 5	2.26	1.92
3 $\bar{1}$ 6	0.60	-0.70
$\bar{3}$ 1 1	6.10	-7.22
$\bar{3}$ 1 2	1.18	-0.74
$\bar{3}$ 1 3	1.78	2.22
$\bar{3}$ 1 4	2.52	-2.94
$\bar{3}$ 1 5	1.44	1.40
$\bar{3}$ 1 6	1.96	1.86
3 2 0	1.42	1.36
3 2 1	15.58	-14.36
3 2 3	3.84	3.62
3 2 4	1.46	1.56

Table 10 (*cont.*)

h k ℓ	F_o	F_c
3 2 $\bar{1}$	3.30	3.76
3 2 $\bar{3}$	8.54	7.04
3 2 $\bar{4}$	2.62	−2.38
3 2 $\bar{5}$	2.52	−2.18
3 2 $\bar{6}$	3.58	3.24
3 2 $\bar{8}$	0.76	−0.68
3 $\bar{2}$ 0	3.00	−2.00
3 $\bar{2}$ 1	5.74	−4.98
3 $\bar{2}$ 2	0.76	0.78
3 $\bar{2}$ 3	4.18	−3.80
3 $\bar{2}$ 5	2.70	2.78
3 $\bar{2}$ 6	0.64	1.04
$\bar{3}$ 2 1	2.70	2.62
$\bar{3}$ 2 2	2.70	−2.10
$\bar{3}$ 2 3	2.96	3.16
$\bar{3}$ 2 4	1.50	1.66
$\bar{3}$ 2 5	0.66	−0.70
3 3 1	4.10	3.96
3 3 2	1.32	1.34
3 3 3	5.14	5.38
3 3 $\bar{1}$	8.10	−11.34
3 3 $\bar{2}$	1.08	1.08
3 3 $\bar{3}$	3.14	2.62
3 3 $\bar{5}$	2.18	2.14
3 3 $\bar{6}$	1.26	−1.36
3 $\bar{3}$ 0	0.60	0.44
3 $\bar{3}$ 1	1.28	1.38
3 $\bar{3}$ 2	3.14	−2.54
3 $\bar{3}$ 3	1.86	−1.88
3 $\bar{3}$ 5	2.18	−1.70
$\bar{3}$ 3 1	3.66	3.66
$\bar{3}$ 3 2	1.20	1.24
$\bar{3}$ 3 3	1.52	−1.38
$\bar{3}$ 3 4	0.96	−0.86
$\bar{3}$ 3 6	0.52	0.44
3 4 0	1.16	1.16
3 4 1	5.40	5.42
3 4 2	0.88	−1.10
3 4 $\bar{1}$	2.36	2.88
3 4 $\bar{3}$	6.44	−5.90
3 4 $\bar{5}$	1.28	1.26
3 $\bar{4}$ 0	1.54	1.54
3 $\bar{4}$ 1	3.04	2.60
3 $\bar{4}$ 2	1.76	1.46
3 $\bar{4}$ 4	2.00	−1.70
$\bar{3}$ 4 1	1.62	−1.52
$\bar{3}$ 4 2	2.24	−1.94
$\bar{3}$ 4 3	0.94	−0.82
$\bar{3}$ 4 4	1.52	1.06
3 5 $\bar{1}$	3.40	3.48
3 5 $\bar{2}$	0.92	1.04
3 5 $\bar{5}$	2.36	−2.34
3 $\bar{5}$ 0	3.22	−2.70
3 $\bar{5}$ 1	1.04	−1.04
3 $\bar{5}$ 2	1.42	1.40
3 $\bar{5}$ 3	1.40	1.58
3 $\bar{5}$ 4	0.94	0.94
3 $\bar{5}$ 5	0.44	−0.28
$\bar{3}$ 5 1	1.08	−0.88
$\bar{3}$ 5 2	1.56	1.32
3 $\bar{6}$ 0	0.90	1.08
3 $\bar{6}$ 1	0.56	−0.74
3 $\bar{6}$ 2	2.36	−2.20
3 $\bar{6}$ 3	0.48	−0.54
3 $\bar{6}$ 4	0.64	0.94
4 0 0	1.24	−1.72
4 0 1	4.88	−5.00
4 0 2	4.62	4.50
4 0 3	1.20	1.72
4 0 4	2.44	−2.84
4 0 5	0.44	−0.24
4 0 $\bar{1}$	3.58	−3.86
4 0 $\bar{2}$	3.66	−3.28
4 0 $\bar{3}$	11.92	11.04
4 0 $\bar{4}$	4.18	3.76
4 0 $\bar{5}$	2.08	−2.02
4 0 $\bar{7}$	2.78	−2.42
4 1 0	5.66	5.54
4 1 1	3.14	2.98
4 1 2	3.40	−3.26
4 1 4	0.34	0.34
4 1 $\bar{1}$	6.18	−6.42
4 1 $\bar{2}$	2.44	−2.62
4 1 $\bar{3}$	2.88	−3.06
4 1 $\bar{4}$	2.20	−2.02
4 1 $\bar{5}$	6.96	6.82
4 1 $\bar{6}$	2.44	2.12
4 1 $\bar{7}$	1.02	−0.98
4 $\bar{1}$ 0	3.30	−3.44
4 $\bar{1}$ 1	3.04	−3.04
4 $\bar{1}$ 2	0.68	−0.64
4 $\bar{1}$ 3	2.18	−2.26
4 $\bar{1}$ 4	2.70	2.50
$\bar{4}$ 1 1	9.84	11.84
$\bar{4}$ 1 2	3.48	4.78
$\bar{4}$ 1 3	2.00	−2.60
$\bar{4}$ 1 5	4.36	−4.78
$\bar{4}$ 1 7	1.96	1.90
4 2 1	1.18	1.38
4 2 3	0.70	0.54
4 2 $\bar{1}$	3.44	3.20
4 2 $\bar{2}$	4.70	4.68
4 2 $\bar{3}$	5.22	−5.00
4 2 $\bar{4}$	2.78	−2.30
4 2 $\bar{5}$	2.18	−2.14
4 2 $\bar{6}$	0.42	−0.62
4 2 $\bar{7}$	3.58	3.10
4 $\bar{2}$ 0	4.44	4.06
4 $\bar{2}$ 1	9.06	8.32
4 $\bar{2}$ 2	2.12	−2.30
4 $\bar{2}$ 3	1.26	−1.72
$\bar{4}$ 2 1	2.00	−2.40
$\bar{4}$ 2 3	5.48	−6.40
$\bar{4}$ 2 4	1.66	−1.68
$\bar{4}$ 2 5	2.70	3.08
4 3 0	0.86	−1.12
4 3 2	1.34	1.46
4 3 $\bar{1}$	1.32	1.48
4 3 $\bar{3}$	2.52	2.42
4 3 $\bar{4}$	2.44	2.60
4 3 $\bar{5}$	2.26	−2.36
4 3 $\bar{6}$	1.48	−1.42
4 3 $\bar{7}$	1.24	−1.30
4 $\bar{3}$ 0	0.62	−0.66
4 $\bar{3}$ 1	2.52	−2.10
4 $\bar{3}$ 2	2.96	2.40
4 $\bar{3}$ 3	4.18	4.06
4 $\bar{3}$ 4	0.72	−0.90
$\bar{4}$ 3 1	5.22	−5.58
$\bar{4}$ 3 2	2.50	−1.82
$\bar{4}$ 3 3	2.70	3.48
$\bar{4}$ 3 5	1.52	1.14
$\bar{4}$ 3 6	1.42	1.18
4 4 0	0.70	0.76
4 4 $\bar{2}$	0.60	−0.84
4 4 $\bar{3}$	0.56	0.74
4 4 $\bar{5}$	1.44	1.46
4 $\bar{4}$ 0	1.36	−1.22
4 $\bar{4}$ 1	3.48	−3.06
4 $\bar{4}$ 2	0.68	−0.86
4 $\bar{4}$ 3	1.56	−1.42
4 $\bar{4}$ 4	1.00	1.08
4 $\bar{4}$ 5	1.30	1.68
$\bar{4}$ 4 1	2.44	2.92
$\bar{4}$ 4 3	1.84	1.26
$\bar{4}$ 4 4	1.70	1.38
4 $\bar{5}$ 0	0.52	0.52
4 $\bar{5}$ 1	2.26	1.96
4 $\bar{5}$ 2	0.52	−0.32
4 $\bar{5}$ 3	0.76	−1.10
4 $\bar{5}$ 4	0.54	−0.78
$\bar{4}$ 5 1	0.52	0.64
$\bar{4}$ 5 2	1.32	1.18
$\bar{4}$ 5 3	0.52	−0.64
5 0 0	4.36	−3.94
5 0 1	1.38	1.58
5 0 2	2.52	2.50
5 0 3	1.50	1.46
5 0 $\bar{1}$	4.96	−5.20
5 0 $\bar{2}$	1.40	−1.08
5 0 $\bar{4}$	3.66	4.08
5 0 $\bar{5}$	1.50	1.46
5 0 $\bar{6}$	1.58	−1.44
5 1 0	2.36	2.20
5 1 1	3.04	2.72
5 1 2	0.60	0.50
5 1 $\bar{1}$	1.62	1.74
5 1 $\bar{2}$	3.30	−3.08
5 1 $\bar{3}$	4.52	−3.94
5 1 $\bar{4}$	1.14	−0.92
5 1 $\bar{6}$	2.44	2.08
5 $\bar{1}$ 0	1.56	−1.56
5 $\bar{1}$ 1	3.74	−4.36
5 $\bar{1}$ 2	2.62	−3.34
5 $\bar{1}$ 3	0.74	1.12
$\bar{5}$ 1 1	0.70	0.66
$\bar{5}$ 1 2	5.06	5.94
$\bar{5}$ 1 3	2.44	2.78
$\bar{5}$ 1 4	2.44	−2.62
$\bar{5}$ 1 6	0.60	−0.74
5 2 0	0.52	0.38
5 2 1	0.74	−0.88
5 2 $\bar{1}$	2.88	2.88
5 2 $\bar{2}$	1.94	1.56
5 2 $\bar{3}$	1.34	1.40
5 2 $\bar{4}$	1.72	−1.52
5 2 $\bar{5}$	2.36	−2.06
5 2 $\bar{6}$	0.98	−0.84
5 $\bar{2}$ 0	6.96	6.22
5 $\bar{2}$ 1	0.88	0.78
5 $\bar{2}$ 2	1.14	−1.68
5 $\bar{2}$ 3	2.88	−2.66
5 $\bar{2}$ 4	1.60	−1.84
$\bar{5}$ 2 1	2.70	3.22
$\bar{5}$ 2 2	2.52	−3.10
$\bar{5}$ 2 3	1.02	−1.02
$\bar{5}$ 2 4	1.84	−1.54
5 3 $\bar{1}$	0.50	−0.90
5 3 $\bar{3}$	1.92	1.74
5 3 $\bar{4}$	1.36	1.12
5 $\bar{3}$ 0	2.62	−2.42
5 $\bar{3}$ 1	3.04	2.46
5 $\bar{3}$ 2	4.70	4.56
5 $\bar{3}$ 3	0.80	0.62
5 $\bar{3}$ 4	0.96	−1.22
$\bar{5}$ 3 1	1.84	−1.48
$\bar{5}$ 3 2	2.90	−2.18
$\bar{5}$ 3 3	0.76	−0.48
$\bar{5}$ 3 4	2.72	2.34
$\bar{5}$ 3 5	1.10	0.72
5 $\bar{4}$ 0	2.04	−2.08
5 $\bar{4}$ 1	1.48	−1.40
5 $\bar{4}$ 2	1.56	−1.44
5 $\bar{4}$ 3	1.62	1.44
$\bar{5}$ 4 1	0.62	−0.42
$\bar{5}$ 4 2	2.26	2.40
$\bar{5}$ 4 3	0.52	−0.32
5 $\bar{5}$ 0	2.08	1.74
5 $\bar{5}$ 2	1.22	−1.28
6 0 1	0.78	0.74
6 0 $\bar{1}$	1.48	1.26
6 0 $\bar{2}$	0.52	−0.46
6 0 $\bar{3}$	0.52	−0.34
6 1 $\bar{3}$	2.00	1.66
$\bar{6}$ 1 2	0.60	0.46
$\bar{6}$ 1 3	0.68	−0.50
$\bar{6}$ 1 4	1.30	−0.96
6 $\bar{2}$ 0	0.60	0.52
6 $\bar{2}$ 1	0.70	−0.70
$\bar{6}$ 2 2	1.18	−0.90
$\bar{6}$ 2 3	1.50	−1.12
$\bar{6}$ 2 4	0.60	0.64
6 $\bar{3}$ 0	0.66	−0.60
6 $\bar{3}$ 1	0.76	0.88
$\bar{6}$ 3 1	1.50	−1.16
$\bar{6}$ 3 2	0.60	0.52

The molecule

Although several amide structures have been reported, few of them have been determined with sufficient accuracy to make a detailed comparison possible. Certain structural similarities are however exhibited, as can be seen below.

	C–N (Å)	C–O (Å)	σ	O–$\hat{C}$–N
Mono fluoroacetamide	1·319	1·254	0·006	124·0
Oxamide [Ayerst & Duke (1954)]	1·315	1·243	0·006	125·7
Succinamide [Davies & Pasternak (1956)]	1·333	1·238	0·002	122·0
Formamide [Ladell & Post (1954)]	1·300	1·255	0·02	121·5

The limits of variation of bond distances in the amide group in these structures are comparatively small, and those found in monofluoroacetamide fall inside these limits. A consistent feature revealed in all determinations is an increase of the angle O–$\hat{C}$–N above 120°.

The C–C bond length of 1·533 Å is only slightly less than that formerly expected for a C–C single bond (1·544 Å). Recent theories [Brown (1959), Dewar & Schmeising (1960)] suggest that this value is to be associated with two carbon atoms with sp^3 hybridization and that a lower value, 1·505 Å, would be expected for Csp^3–Csp^2. If these newer ideas are valid, there is a lengthening of the C–C bond in mono fluoro-acetamide. Other amides show a lengthening of the C–C bond compared with the values suggested by Brown, Dewar & Schmeising. For instance, in oxamide the C–C bond is 1·542 Å compared with the value 1·470 Å expected for Csp^2–Csp^2. This may be attributed to a disturbance of the perfectly symmetrical trigonal hybridization at the amide carbon. If the orbital in the C–C direction has less *s* and more *p* character than the other two orbitals, there will be an increase in the effective C amide 'radius' in this direction and an increase in the angle O–C–N above 120° on account of the greater *s* character in C–O and C–N bonds. The effective C amide sp^2 'radius' away from the amide group may then be estimated as half of the C–C distance in oxamide i.e. 0·771 Å. Application of this value to mono-fluoroacetamide leads to an expected value of C–C as 1·543 Å if the Csp^3 'radius' is accepted as 0·772 Å. (This may however be influenced by the presence of the fluorine atom and is contingent upon the validity of the conclusions of Dewar & Schmeising).

Carbon–fluorine distances in other molecules range from 1·313 Å to 1·391 Å. Bent (1960) has summarized these and related them to the electronegativity of the group attached to the fluorine atom, the shorter distances being associated with increased electronegativity of the attached group. The C–F distance, 1·406 Å, found in monofluoroacetamide indicates on this basis more polarity in the C–F bond and a decrease in *s* character in the C orbital in the C–F direction; this would be consistent with the shortening of the C–C bond discussed above.

An unexpected feature of the molecule is the close planarity of the atoms F, C_1, C_2, O, N (Table 9); if this were a chance coincidence of the packing of the molecules it would be unlikely to be so exactly planar. That the planarity is not due to Coulombic repulsion of the electronegative O and F atoms may be deduced from the greater O–F distance within the molecule, 3·547 Å, compared with 3·470 Å between neighbouring molecules. The existence of an intramolecular attraction between the fluorine atom and the amide nitrogen or hydrogen is strongly suggested; a similar intramolecular attraction between hydroxyl and carbonyl oxygen atoms has already been postulated by Jeffrey & Parry (1952).

That the attraction is a strong one in monofluoroacetamide is shown by the fact that the F–F''' intermolecular repulsion causes a tilt of the molecules from the plane of hydrogen bonding in preference to a twist of the CH_2F group about the C–C bond.

We are indebted to those authors mentioned in this paper whose computer programmes we have used freely; in particular we thank Dr J. S. Rollett for the use of the MERCURY computer at Oxford University and for a great deal of helpful advice on the least-squares refinement. We are grateful to the Department of Scientific and Industrial Research for the award of a Research Grant to one of us (D. O. H.) and for the provision of a grant to enable the computational work to be carried out.

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