represented by the dotted line (*b*). The value $\Theta_{T_r}=$ 191 °K. for $T_r=293$ °K. as determined by Spreadborough & Christian (1959) gives according to relation (3) the temperature dependence of Θ indicated in Fig. 4 by a curve (*c*). It can be seen that the $\Theta(T)$-curves obtained from X-ray data by various authors differ considerably. For this reason three different procedures were used in our paper for deriving $\Theta(T)$-dependence from X-ray measurements. The resulting Θ_T-values obtained from our measurements applying (A) are given in Fig. 4 by circles, and in the same figure the $\Theta(T)$-curves resulting from (B)(i) and (B)(ii) are represented by the lines (*d*) and (*e*) respectively. Fig. 4 shows that all three procedures yield practically identical $\Theta(T)$-curves. The reliability of our measurements can be demonstrated especially by the agreement of the results obtained by assuming the knowledge of the scattering curve of the atom at rest in (A) and on the other hand by assuming the change of Θ with temperature according to Grüneisen's law in (B)(i), which is thus closely obeyed by silver up to the temperature of about 900 °K. The value of $\Theta_0=$ 218 °K. for $T=0$ °K. obtained by extrapolation in the curve resulting from (B)(i) is also sufficiently close to the value of $\Theta_0=225{\cdot}3$ °K. deduced from specific-heat measurements (Corak, Garfunkel, Satterthwaite & Wexler, 1955).

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References

Andriessen, R. (1935). *Physica*, **2**, 417.
Blackman, M. (1955). *Handbuch der Physik*, Vol. VII/1, *Kristallphysik*, p. 335. Berlin: Springer.
Boskovits, J., Roilos, M., Theodossiou, A. & Alexopulos, K. (1958). *Acta Cryst.* **11**, 845.
Corak, W. S., Garfunkel, M. P., Satterthwaite, C. B. & Wexler, A. (1955). *Phys. Rev.* **98**, 1699.
Černohorský, M. (1959). *Práce Brněnské základny ČSAV*, spis 384, **31**, 130.
James, R. W. (1954). *The Optical Principles of the Diffraction of X-rays*, p. 193. London: Bell.
Paskin, A. (1957). *Acta Cryst.* **10**, 667.
Reynolds, P. W. & Hume-Rothery, W. (1938). *Proc. Roy. Soc.* A, **167**, 25.
Sagel, K. (1958). *Tabellen zur Röntgenstrukturanalyse*. Berlin: Springer.
Simerská, M. & Syneček, V. (1959). *Czech. J. Phys.* **9**, 395.
Spreadborough, J. & Christian, J. W. (1959*a*). *Proc. Phys. Soc.* **74**, 609.
Spreadborough, J. & Christian, J. W. (1959*b*). *J. Sci. Instrum.* **36**, 116.

Acta Cryst. (1961). **14**, 1262

X-ray Studies of Molecular Overcrowding. II. The Crystal and Molecular Structure of *o*-Chlorobenzoic Acid

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o-Chlorobenzoic acid crystallizes in the monoclinic system, space group $C2/c$, with eight molecules in a unit cell of dimensions

$$a=14{\cdot}73,\quad b=3{\cdot}90,\quad c=25{\cdot}50\ \text{Å},\quad \beta=112°\ 40'.$$

The crystal structure, which consists of centrosymmetrical hydrogen-bonded dimers, was elucidated initially in projection. The final atomic parameters were obtained from a least-squares treatment of the three-dimensional data, a total of 1034 observed structure factors being employed. The strain which would be imposed on a planar ideal molecule is relieved in a number of ways.

(i) The carboxyl group is rotated about the exocyclic C–C bond 13·7° out of the plane of the benzene ring.

(ii) The chlorine atom and the exocyclic carbon atom are displaced +0·036 and −0·058 Å, respectively, out of the plane of the benzene ring.

(iii) The exocyclic C–C and C–Cl bonds are displaced sideways so that the normal valency angles of 120° are increased to 122·5° and 124·7°, respectively.

1. Introduction

That steric interactions between adjacent non-bonded atoms may have an appreciable effect on molecular properties such as ultra-violet absorption has long been recognized and an extensive literature exists concerning both experimental and theoretical aspects of the subject. See, for example, Gray (1958).

Descriptions have been published of the molecular structures of a number of overcrowded compounds. For aromatic hydrocarbons it appears that theoretical calculations (Coulson & Senent, 1955) can yield deviations from planarity which are in agreement with those determined experimentally (McIntosh, Robertson & Vand, 1954). The situation with polyhalogenobenzene derivatives is not so clear: experimental results obtained by different methods are often inconsistent and theoretical models do not yet appear to be sufficiently precise (Gafner & Herbstein, 1960; Coulson & Stocker, 1959). Moreover, the accurate location of the lighter atoms in such molecules is difficult and a really detailed description of the structure may still be impossible even when the positions of the halogen atoms have been accurately determined.

Monohalogenobenzene derivatives subject to steric effects because of the close proximity of the halogen atom to a neighbouring group offer a greater prospect of locating the lighter atoms accurately and in the course of a study of overcrowded benzoic acids we have carried out crystal-structure analyses of several halogenobenzoic acids. The present paper gives an account of the investigation of *o*-chlorobenzoic acid. To ensure significant results three-dimensional X-ray diffraction data have been utilized.

2. Crystal data

o-Chlorobenzoic acid, $C_7H_5O_2Cl$; *M*, 156·6; m.p. 142 °C.;

d, calc. 1·539, meas. 1·544 g.cm.$^{-3}$ (Steinmetz, 1914). Monoclinic,

$$a = 14{\cdot}73 \pm 0{\cdot}03,\ b = 3{\cdot}90 \pm 0{\cdot}02,\ c = 25{\cdot}50 \pm 0{\cdot}05\ \text{Å},\ \beta = 112^\circ\ 40' \pm 20'.$$

Space group deduced from absent reflexions either $Cc\text{–}C_s^4$ or $C2/c\text{–}C_{2h}^6$. Structure refinement confirms $C2/c$ as true space group. Eight molecules per unit cell. Volume of the unit cell, 1351 Å^3. Absorption coefficient for X-rays, $\lambda = 1{\cdot}542$ Å, $\mu = 44{\cdot}8$ cm.$^{-1}$. Total number of electrons per unit cell $= F(000) = 640$.

Crystallization from acetone solution gave single crystals of *o*-chlorobenzoic acid in the form of thin, narrow laths elongated along *b*. The morphology has been described by Steinmetz (1914), whose axial ratios, 3·782:1:6·625, $\beta = 112^\circ\ 40'$, differ slightly from ours (3·777:1:6·539).

3. Experimental

Rotation, oscillation and moving-film photographic methods were used, with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}542$ Å). The cell dimensions were determined from rotation and equatorial layer line Weissenberg photographs. The

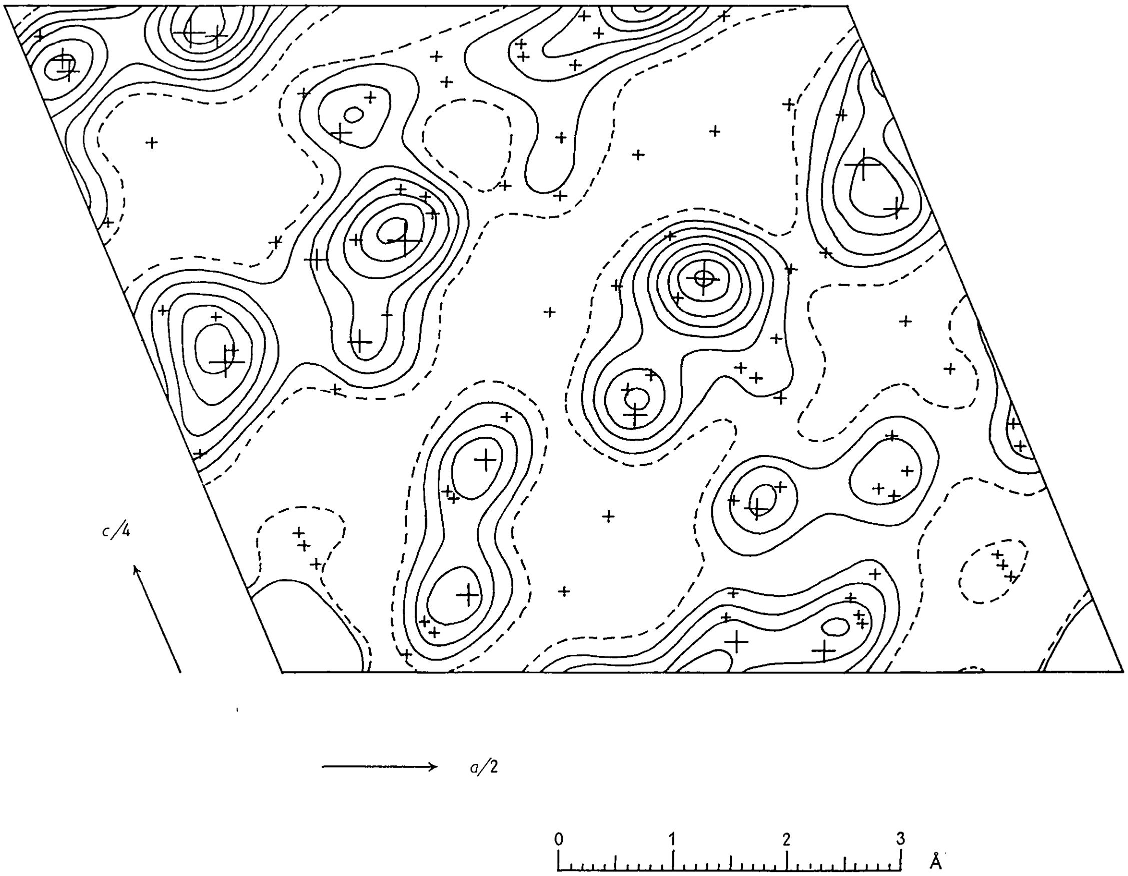


Fig. 1. Patterson projection along the *b* axis. Contours at equal arbitrary intervals, the lowest contour being broken. The interatomic vectors are marked by crosses.

intensity data were obtained from multiple-film equi-inclination Weissenberg photographs of the $h0l$, $h1l$, $h2l$ and $h3l$ layers. The number of independent reflexions observed was 1034. The intensities were corrected for Lorentz, polarization, and the rotation factors appropriate to upper layers (Tunell, 1939). Small crystals of uniform cross-section were employed and no absorption corrections were applied. The scaling factor for each layer was adjusted during refinement to ensure that $\Sigma|F_o|=\Sigma|F_c|$. The values of the measured structure amplitudes on the final, absolute, scale are listed in Table 8.

4. Structure determination

The b-axis projection

At the outset it seemed probable that the *o*-chlorobenzoic acid molecules would occur as centrosymmetrical dimers in the crystal, with hydrogen bonding between the adjacent carboxyl groups. The space group was assumed, therefore, to be $C2/c$ and not Cc. This assumption was later justified by the agreement obtained between measured and calculated structure factors.

Because of the short length of the b axis it was apparent that good resolution of the atoms would be obtained in the projection along this axis. From a Patterson projection (Fig. 1) approximate positions for the chlorine, carbon and oxygen atoms were obtained and were subsequently refined by Fourier and least-squares techniques. In the structure-factor calculations the atomic form factors employed were those of Berghuis *et al.* (1955) for carbon and oxygen, those of Tomiie & Stam (1958) for chlorine and those of McWeeny (1951) for hydrogen. After a number of cycles the value of R, the usual discrepancy factor, fell to 0·108 and the parameter shifts became extremely small.

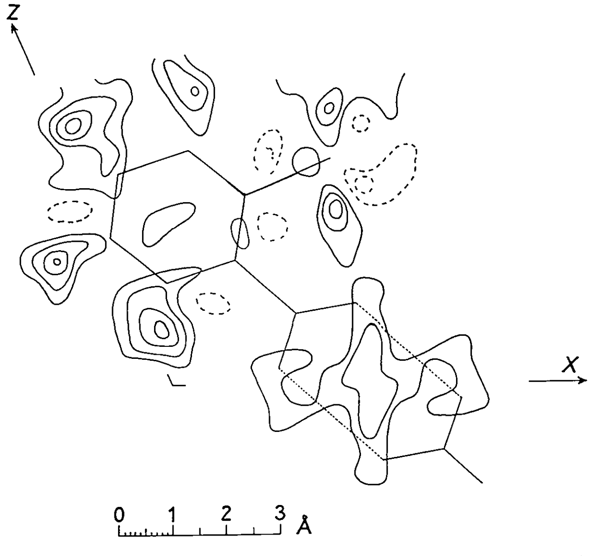


Fig. 2. Difference-synthesis projection on (010) to show the electron distribution due to the hydrogen atoms. Contours at intervals of 0·2 e.Å^{-2}, negative contours broken, zero contour omitted.

When the hydrogen atoms were omitted from the structure-factor calculations the value of R increased to 0·124. With the values of $(F_o-F_{c'})$ a difference map was computed (Fig. 2). It represents the difference between the electron distribution existing in the crystal and that calculated for chlorine, oxygen and carbon atoms only, at their appropriate positions in the unit cell and with their appropriate thermal vibrations. On this map there are a number of significant peaks which are clearly due to the hydrogen atoms. The hydrogen atom of the carboxyl group, responsible for the hydrogen-bonding which exists between the two adjacent molecules, shows up less well than the hydrogen atoms attached to the carbon atoms of the benzene ring. Similar results were observed in salicylic acid (Cochran, 1953) and in benzoic acid (Sim, Robertson & Goodwin, 1955) and are probably connected with the partial ionization of the hydrogen atom of the carboxyl group.

Three-dimensional refinement

During the course of the refinement of the b-axis projection of *o*-chlorobenzoic acid a study of *o*-bromobenzoic acid was begun. As the two acids proved to be isomorphous it was possible to use the y-coordinates deduced for the atoms of *o*-bromobenzoic acid as the starting point for the detailed three-dimensional refinement of *o*-chlorobenzoic acid. With these y-coordinates, the x- and z-coordinates of the two-dimensional refinement and an isotropic temperature factor B of 4·0 Å^2 for all atoms including hydrogen, structure factors were calculated for the $h2l$ and $h3l$ reflexions and R values of 0·300 and 0·360 obtained. Difference Fourier line syntheses led to improved y-coordinates for the chlorine, carbon and oxygen atoms and lower values of R, 0·174 for the $h1l$, 0·200 for the $h2l$ and 0·263 for the $h3l$ reflexions.

The good measure of agreement between measured and calculated structure amplitudes at this stage indicated that the coordinates were sufficiently accurate to warrant proceeding to a least-squares refinement of both positional and anisotropic temperature-factor parameters for all atoms other than hydrogen. In the least-squares analysis 223 unobserved terms were included, each with a value of $|F_o|$ equal to one-half of the minimum $|F|$ locally observable. After six rounds of calculations the parameter shifts became negligible and the values of R were reduced to 0·090 for the $h0l$, 0·098 for the $h1l$, 0·109 for the $h2l$ and 0·167 for the $h3l$ reflexions. The overall final value of R for the 1034 observed reflexions is 0·105.

The final calculated and measured structure factors are listed in Table 8.

5. Coordinates, molecular dimensions and estimates of accuracy

The final coordinates of the carbon, oxygen and chlorine atoms and the final anisotropic temperature-factor parameters are shown in Tables 1 and 2 respectively. The standard deviations of the positional parameters, calculated by the standard method from the final least-squares analysis, are given in Table 3. From these results the estimated standard deviation of a C–C bond is about 0·009 Å, that of a C–O bond is about 0·008 Å, and that of the C–Cl bond is 0·007 Å. The estimated standard deviation of bond angles is 0·6°.

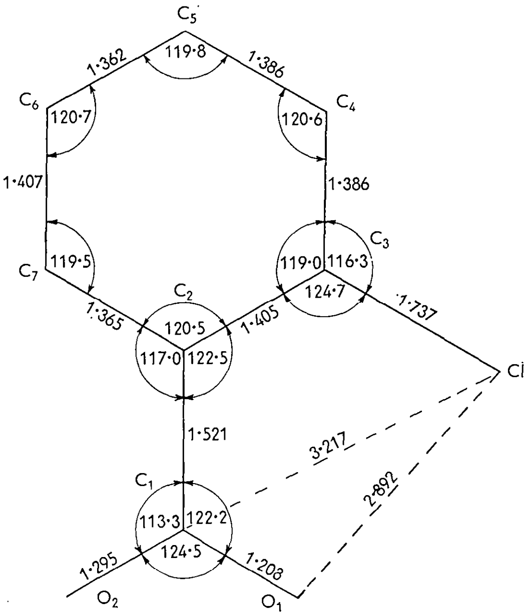


Fig. 3. Interatomic distances and valency angles in *o*-chlorobenzoic acid.

Table 1. *Final atomic coordinates*

Coordinates x, y, z are referred to the monoclinic crystal axes and are expressed as fractions of the axial lengths, with origin at the centre of symmetry on glide plane c. Coordinates X', Y and Z' are referred to orthogonal axes a, b, and c', c' being taken perpendicular to the a and b crystal axes, and are expressed in Å units

Atom	x	y	z	X'	Y	Z'
C_1	0·1961	0·3430	0·0550	2·347	1·338	1·295
C_2	0·1480	0·4213	0·0969	1·228	1·643	2·280
C_3	0·1997	0·5710	0·1503	1·465	2·227	3·537
C_4	0·1498	0·6447	0·1852	0·386	2·514	4·358
C_5	0·0501	0·5751	0·1676	−0·910	2·243	3·943
C_6	0·0009	0·4282	0·1159	−1·126	1·670	2·726
C_7	0·0501	0·3488	0·0798	−0·047	1·360	1·878
O_1	0·2760	0·4551	0·0610	3·465	1·775	1·435
O_2	0·1427	0·1498	0·0132	1·973	0·584	0·310
Cl	0·3247	0·6642	0·1775	3·038	2·591	4·176

Table 3. *Estimated standard deviations in atomic coordinates*

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
C_1	0·0049 Å	0·0076 Å	0·0053 Å
C_2	0·0050	0·0064	0·0051
C_3	0·0058	0·0065	0·0055
C_4	0·0062	0·0079	0·0061
C_5	0·0062	0·0073	0·0061
C_6	0·0057	0·0082	0·0061
C_7	0·0054	0·0080	0·0057
O_1	0·0039	0·0055	0·0043
O_2	0·0039	0·0052	0·0039
Cl	0·0015	0·0022	0·0015

Table 4. *The shorter intermolecular contacts*

$O_1 \cdots O_2^{I}$	2·632 Å	$C_4 \cdots C_7^{II}$	3·726 Å
$O_1 \cdots O_2^{II}$	3·291	$C_5 \cdots C_7^{II}$	3·757
$O_1 \cdots O_1^{I}$	3·315	$C_4 \cdots C_2^{II}$	3·769
$C_1 \cdots O_2^{II}$	3·318	$C_3 \cdots C_7^{II}$	3·773
$C_1 \cdots O_1^{I}$	3·349	$C_4 \cdots C_6^{II}$	3·780
$C_1 \cdots O_2^{I}$	3·443	$Cl \cdots C_5^{V}$	3·781
$C_7 \cdots O_2^{III}$	3·504	$C_1 \cdots C_1^{I}$	3·791
$C_7 \cdots O_2^{IV}$	3·510	$C_6 \cdots C_7^{II}$	3·844
$C_2 \cdots O_2^{II}$	3·536	$C_2 \cdots C_7^{II}$	3·856
$C_5 \cdots C_6^{II}$	3·550	$C_3 \cdots C_1^{II}$	3·856
$C_3 \cdots C_2^{II}$	3·555	$C_4 \cdots C_3^{II}$	3·859
$C_6 \cdots O_2^{IV}$	3·556	$Cl \cdots C_4^{VIII}$	3·859
$O_2 \cdots O_2^{I}$	3·563	$C_4 \cdots C_5^{II}$	3·875
$O_1 \cdots C_6^{V}$	3·573	$C_6 \cdots O_2^{III}$	3·875
$O_1 \cdots C_1^{II}$	3·642	$C_2 \cdots C_1^{II}$	3·892
$Cl \cdots C_6^{V}$	3·662	$C_7 \cdots C_7^{IV}$	3·937
$C_6 \cdots O_1^{VII}$	3·686	$C_4 \cdots C_4^{VIII}$	3·990
$O_1 \cdots O_1^{VI}$	3·704		

The superscripts refer to the following positions

I	$\frac{1}{2}-x$	$\frac{1}{2}-y$	$-z$
II	x	$1+y$	z
III	$-x$	$-y$	$-z$
IV	$-x$	$1-y$	$-z$
V	$\frac{1}{2}+x$	$\frac{1}{2}+y$	z
VI	$\frac{1}{2}-x$	$1\frac{1}{2}-y$	$-z$
VII	$x-\frac{1}{2}$	$\frac{1}{2}+y$	z
VIII	$\frac{1}{2}-x$	$\frac{1}{2}+y$	$\frac{1}{2}-z$

Table 2. *Anisotropic temperature-factor parameters*

Atom	B_{hh}	B_{kk}	B_{ll}	B_{kl}	B_{hl}	B_{hk}
C_1	0·00608	0·12749	0·00265	−0·00738	0·00381	−0·00283
C_2	0·00734	0·10160	0·00233	−0·00060	0·00442	0·00529
C_3	0·00983	0·09792	0·00256	0·00024	0·00498	0·01457
C_4	0·01026	0·12289	0·00325	−0·00447	0·00518	0·01064
C_5	0·01106	0·12716	0·00312	−0·00138	0·00626	0·01384
C_6	0·00799	0·18327	0·00330	0·00095	0·00574	0·00826
C_7	0·00740	0·13293	0·00317	−0·00375	0·00429	0·00570
O_1	0·00836	0·19388	0·00398	−0·01820	0·00590	−0·01236
O_2	0·01033	0·16397	0·00316	−0·01678	0·00561	−0·01131
Cl	0·00866	0·15218	0·00265	−0·00879	0·00458	−0·01104
Isotropic $B=4·0$ Å^2 (Hydrogen atoms)	0·00780	0·09485	0·00260	—	0·00347	—

The temperature factor is expressed in the form

$$2^{-(B_{hh}h^2+B_{kk}k^2+B_{ll}l^2+B_{kl}kl+B_{hl}hl+B_{hk}hk)}$$

The bond lengths and valency angles in the molecule were calculated from the coordinates of Table 1 and are shown in Fig. 3. The shorter intermolecular contacts are listed in Table 4.

The best plane through the chlorine, carbon and oxygen atoms of the molecule, derived by the method of Schomaker *et al.* (1959) is

$$0{\cdot}09504X' - 0{\cdot}90257Y + 0{\cdot}41992Z' + 0{\cdot}41813 = 0\ .$$

The deviations of the atoms from this plane (Table 5) show that the molecule is clearly non-planar. As the oxygen atoms are the main cause of non-planarity the best plane through the chlorine and carbon atoms was calculated. The equation of this plane is

$$0{\cdot}06636X' - 0{\cdot}91457Y + 0{\cdot}39895Z' + 0{\cdot}52237 = 0\ .$$

The deviations of the atoms from this plane (Table 5) are still large ($\Sigma\Delta^2 = 2{\cdot}48 \times 10^{-3}$ Å^2) and since

$$\chi^2 = \Sigma\Delta^2/\sigma^2 \approx 50$$

they must be regarded as highly significant (Fisher & Yates, 1957). This suggests that the chlorine atom and the exocyclic carbon atom are displaced from the plane of the benzene ring. Accordingly, the best plane through only the carbon atoms of the benzene ring was calculated, the equation obtained being

$$0{\cdot}06604X' - 0{\cdot}90890Y + 0{\cdot}41176Z' + 0{\cdot}47017 = 0\ .$$

Displacements from this plane are shown in Table 5. For the benzene ring atoms the deviations are small ($\Sigma\Delta^2 = 7{\cdot}48 \times 10^{-5}$ Å^2) and since

$$\chi^2 \approx 1{\cdot}5$$

the displacements are not significant.

Table 5. *Deviations from the mean planes*

(*a*) Plane through $C_1 \cdots C_7$, O_1, O_2, Cl
(*b*) Plane through $C_1 \cdots C_7$, Cl
(*c*) Plane through benzene ring atoms $C_2 \cdots C_7$
(*d*) Plane through C_1, C_2, O_1, O_2

Atom	(*a*)	(*b*)	(*c*)	(*d*)
C_1	−0·022 Å	−0·029 Å	−0·058 Å	0·003 Å
C_2	0·009	0·011	−0·004	−0·001
C_3	0·033	−0·006	−0·001	—
C_4	0·016	−0·013	0·005	—
C_5	−0·037	−0·016	−0·005	—
C_6	−0·052	0·008	0·000	—
C_7	−0·026	0·024	0·004	—
O_1	−0·252	−0·299	−0·323	−0·001
O_2	0·209	0·243	0·197	−0·001
Cl	0·123	0·021	0·036	—

The atoms of the carboxyl group (C_1, O_1 and O_2) and carbon atom C_2 of the benzene ring lie on the plane

$$0{\cdot}24764X' - 0{\cdot}81107Y + 0{\cdot}52994Z' - 0{\cdot}18001 = 0\ .$$

The angle between the plane of the carboxyl group and the plane of the benzene ring is 13·7°.

6. Location of the hydrogen atoms

The section through the three-dimensional electron-density distribution evaluated in the plane of the benzene ring is shown in Fig. 4. The quarter-electron contour provides distinct evidence of the hydrogen atoms attached to the carbon atoms of the benzene ring. To provide a more detailed picture a triple $(F_o - F_{c'})$ synthesis was computed in the plane of the

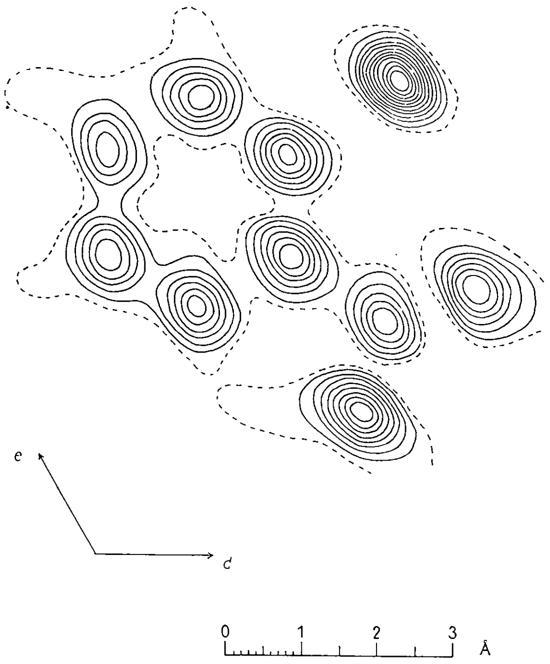


Fig. 4. A section through the plane of the carbon atoms of the benzene ring. The chlorine atom, exocyclic carbon atom and the oxygen atoms are out of this plane. The lowest contour (broken) is 0·25 e.Å^{-3}. Thereafter the contours around the carbon and oxygen atoms are at 1, 2, 3 e.Å^{-3}, etc. while those around the chlorine atom are at 2, 4, 6 e.Å^{-3}, etc.

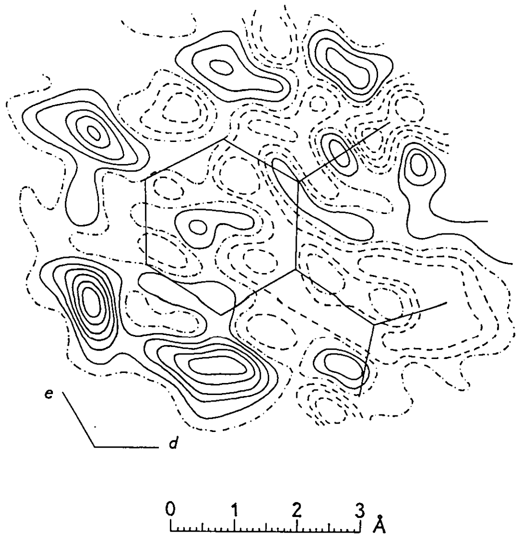


Fig. 5. Difference synthesis in the plane of the benzene ring to show the hydrogen atoms. Contour interval 0·1 e.Å^{-3} with negative levels broken.

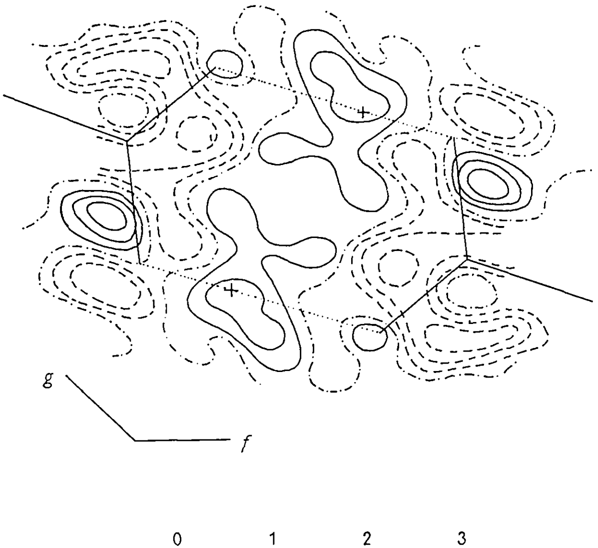


Fig. 6. Difference synthesis in the oxygen plane to show the hydrogen atom of the carboxyl group. Contour interval 0·1 e.Å^{-3}, negative levels broken, zero contour dotted.

benzene ring. Here $F_{c'}$ is the calculated value of the structure factor for the chlorine, carbon and oxygen atoms alone. The result is shown in Fig. 5 where the hydrogen atoms appear as well-resolved peaks of from about 0·32 e.Å^{-3} to 0·66 e.Å^{-3} in height.

The C–H bond lengths measured directly on this map are given in Table 6. The average value is 1·01 Å.

In an attempt to locate the hydrogen atom which is responsible for hydrogen bonding in the dimer a triple $(F_o - F_{c'})$ synthesis was computed in the plane through the four oxygen atoms O_1, O_2, O_1' and O_2' and the centre of symmetry at $(\frac{1}{4}, \frac{1}{4}, 0)$. The result is shown in Fig. 6. The expected position of the hydrogen atom, on the dotted line joining the oxygen atoms, is indicated by a cross at 1·0 Å from the oxygen atom O_2. The actual hydrogen peak, a somewhat diffuse peak of about 0·27 e.Å^{-3} in height, is in reasonable agreement with this assignment.

Table 6. *Carbon–hydrogen bond lengths*

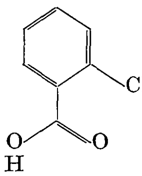
H–C_4	1·11 Å	H–C_6	1·00 Å
H–C_5	1·09	H–C_7	0·85

7. Discussion

The Cl · · · O_1 (2·892 Å) and Cl · · · C_1 (3·217 Å) intramolecular separations are appreciably shorter than the sums of the van der Waals radii (3·20 Å and 3·80 Å respectively). The molecule may therefore be expected to be subject to some strain.

The displacements of the carbon atoms of the benzene ring from a plane (Table 5) vary from zero to 0·005 Å. These are not significant and the ring may be assumed strictly planar. The displacements of the atoms C_1 and Cl from the benzene plane are −0·058 Å and +0·036 Å respectively. These displacements, though small, are several times greater than the standard deviation of position of the atoms concerned and are significant (see § 5). They correspond to the C–Cl bond and the exocyclic C–C bond bending in opposite directions out of the plane of the benzene ring through angles of 1·2° and 2·2° respectively. The rotation of the carboxyl group around the exocyclic C–C bond so that the angle between the planes of the carboxyl group and the aromatic ring is 13·7° and the significant in-plane displacements of the C–Cl and exocyclic C–C bonds away from one another so that two of the exocyclic valency angles are increased from the normal value of 120° to 122·5° and 124·7° while the adjacent angles are decreased to 117·0° and 116·3° (Fig. 3) must also contribute towards relieving the strain.

In the benzene ring there is some indication of the bonds alternating in length around the ring. Thus the mean length of the bonds C_2–C_3, C_4–C_5 and C_6–C_7 is 1·399 Å whereas the mean length of the bonds C_3–C_4, C_5–C_6 and C_7–C_2 is 1·371 Å, a difference of 0·028 Å. In view of the low estimated standard deviation of bond length obtained in the analysis this bond-fixation effect is probably significant. It can be attributed to repulsion between the adjacent chlorine atom and carboxyl group (in particular C_1) causing the Kekulé structure (I) to be rather more favoured energetically than the alternative structure (II) and these, therefore, do not contribute equally to the molecular structure.



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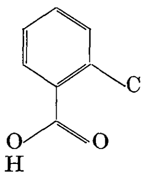

II

The exocyclic C_2–C_1 bond leading to the carboxyl group is 1·521 Å in length. The standard single-bond distance between carbon atoms in the sp^2 state of hybridization has been estimated (Dewar & Schmeising, 1959) as 1·479 Å, close to the values in butadiene, 1·483 Å, *p*-benzoquinone, 1·477 Å (Trotter, 1960), benzoic acid, 1·48 Å, and salicylic acid, 1·458 Å. The value of 1·521 Å found in the present analysis is closer to the length of the central bond in oxalic acid dihydrate, 1·53 Å (Ahmed & Cruickshank, 1953) and the mean length of the *peri*-bonds in quaterrylene, 1·53 Å (Shrivastava & Speakman, 1960). That the *peri*-bonds in the latter molecule are longer than might have been expected has been attributed to repulsion between overcrowded hydrogen atoms and to the *cis*-interactions of C–C bonds. The length of the exocyclic C–C bond in *o*-chlorobenzoic acid is probably similarly related to the intramolecular overcrowding.

In the carboxyl group the mean C–O distance of 1·252 Å is a little shorter than the means of 1·287 Å in succinic acid (Broadley, Cruickshank, Morrison, Robertson & Shearer, 1959) and 1·285 Å in salicylic acid and is rather closer to the means of 1·261 Å in L-serine phosphate (McCallum, Robertson & Sim, 1959), 1·24 Å in α-oxalic acid (Cox, Dougill & Jeffrey, 1952) and 1·24 Å in oxalic acid dihydrate. It is perhaps relevant that, as in *o*-chlorobenzoic acid, the latter group of acids involves C–C bonds from the carboxyl groups somewhat longer than expected, whereas in succinic acid and salicylic acid these bonds (1·485 Å and 1·458 Å) are rather shorter than expected.

Table 7. *Angles about the carbon atom of the carboxyl group in some carboxylic acids*

	∠ CCO	∠ CC(OH)	∠ OC(OH)
o-Chlorobenzoic acid	122·2°	113·3°	124·4°
Succinic acid	124·4	112·9	122·7
Salicylic acid	122·7	117·0	120·2
L-Serine phosphate	121·1	113·5	125·3
Oxalic acid dihydrate	121·6	112·6	125·8

The angles around the carbon atom of the carboxyl group conform to the pattern observed in other carboxylic acids (see Table 7). Invariably the angle CC(OH) is approximately tetrahedral whereas the angles CCO and OC(OH) exceed 120°.

The C–Cl distance of 1·737 Å is significantly shorter than the mean C–Cl distance in halogenated aliphatic compounds, 1·767 Å (*Tables of Interatomic Distances*, 1958). The contraction of 0·03 Å is equal to the expected decrease in radius of a carbon atom on changing from sp^3 to sp^2 hybridization. This suggests that there is little, if any, double-bond character associated with the carbon–halogen bond.

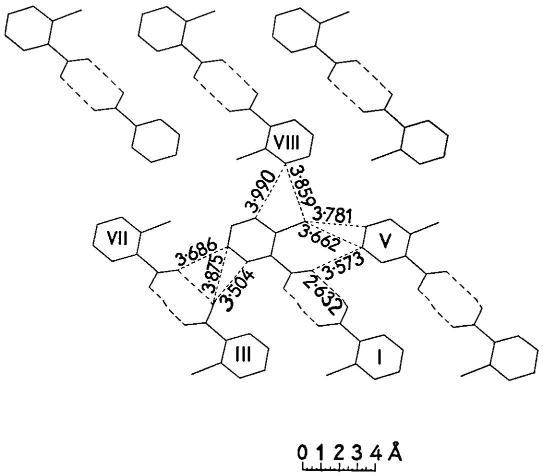

Fig. 7. Arrangement of molecules in the (010) projection.

The arrangement of the molecules in the *b*-axis projection is shown in Fig. 7. The shortest intermolecular contact occurs between oxygen atoms of the carboxyl group. The OH · · · O distance here is 2·63 Å which is normal for this type of hydrogen bonding. All other intermolecular approach distances (Table 4 and Fig. 7) are greater than 3 Å and correspond to normal van der Waals interactions.

The numerical calculations were carried out on the Glasgow University DEUCE computer using programmes devised by Dr J. S. Rollett and Dr J. G. Sime and we are indebted to the Director of the Computing Laboratory, Dr D. C. Gilles, and his staff for facilities. We wish to express our thanks to Prof. J. M. Robertson, F.R.S., for his interest and to the Carnegie Trust for the award of a scholarship which enabled G. F. to participate in this work.

References

Ahmed, F. R. & Cruickshank, D. W. J. (1953). *Acta Cryst.* **6**, 385.

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B. O., MacGillavry, C. H. & Veenendaal, A. L. (1955). *Acta Cryst.* **8**, 478.

Broadley, J. S., Cruickshank, D. W. J., Morrison, J. D., Robertson, J. M. & Shearer, H. M. M. (1959). *Proc. Roy. Soc.* A, **251**, 441.

Cochran, W. (1953). *Acta Cryst.* **6**, 260.

Coulson, C. A. & Senent, S. (1955). *J. Chem. Soc.* p. 1819.

Coulson, C. A. & Stocker, D. (1959). *Mol. Phys.* **2**, 397.

Cox, E. G., Dougill, M. W. & Jeffrey, G. A. (1952). *J. Chem. Soc.* p. 4854.

Dewar, M. J. S. & Schmeising, H. N. (1959). Tetrahedron, **5**, 166.

Fisher, R. A. & Yates, F. (1957). *Statistical Tables.* Edinburgh: Oliver and Boyd.

Gafner, G. & Herbstein, F. H. (1960). *Acta Cryst.* **13**, 706.

Gray, G. W. (1958). *Steric Effects in Conjugated Systems.* London: Butterworths.

McCallum, G. H., Robertson, J. M. & Sim, G. A. (1959). *Nature, Lond.* **184**, 1863.

McIntosh, A. D., Robertson, J. M. & Vand, V. (1954). *J. Chem. Soc.* p. 1661.

McWeeny, R. (1951). *Acta Cryst.* **4**, 513.

Schomaker, V., Waser, J., Marsh, R. E. & Bergman, G. (1959). *Acta Cryst.* **12**, 600.

Shrivastava, H. N. & Speakman, J. C. (1960). *Proc. Roy. Soc.* A, **257**, 477.

Sim, G. A., Robertson, J. M. & Goodwin, T. H. (1955). *Acta Cryst.* **8**, 157.

Steinmetz, H. (1914). *Z. Kristallogr.* **53**, 485.

Tables of Interatomic Distances and Configuration in Molecules and Ions (1958). London: The Chemical Society.

Tomiie, Y. & Stam, C. H. (1958). *Acta Cryst.* **11**, 126.

Trotter, J. (1960). *Acta Cryst.* **13**, 86.

Tunell, G. (1939). *Amer. Min.* **24**, 448.

Table 8. *Calculated and measured structure factors*

h	k	l	F(calc)	F(meas)
0	0	4	-100.9	77.6
0	0	6	101.5	90.7
0	0	8	-133.5	120.0
0	0	10	14.4	15.5
0	0	12	81.6	70.8
0	0	14	-47.4	44.9
0	0	16	37.5	34.1
0	0	18	31.5	30.9
0	0	20	-19.3	19.2
0	0	22	17.4	15.6
0	0	24	-11.3	10.7
0	0	26	-15.3	15.7
0	0	28	7.0	< 3.2
0	0	30	-9.2	< 2.0
2	0	-30	-4.1	< 3.0
2	0	-28	-0.4	< 4.0
2	0	-26	27.6	28.3
2	0	-24	13.8	19.2
2	0	-22	7.8	< 4.9
2	0	-20	3.6	< 4.7
2	0	-18	-37.1	31.8
2	0	-16	14.6	12.4
2	0	-14	34.0	33.8
2	0	-12	-14.1	11.2
2	0	-10	88.5	84.2
2	0	-8	77.9	79.4
2	0	-6	-52.8	63.2
2	0	-4	35.8	43.7
2	0	-2	56.0	49.5
2	0	0	-112.0	108.3
2	0	2	-74.9	72.8
2	0	4	-106.5	104.8
2	0	6	-44.3	44.5
2	0	8	84.8	71.7
2	0	10	2.2	< 3.4
2	0	12	-10.9	13.0
2	0	14	-20.4	23.3
2	0	16	-51.5	53.0
2	0	18	9.2	< 4.8
2	0	20	-10.9	< 4.9
2	0	22	-32.6	34.5
2	0	24	18.6	17.3
2	0	26	2.8	< 3.7
2	0	28	-7.2	< 2.6
4	0	-30	14.6	13.6
4	0	-28	-10.8	8.3
4	0	-26	5.2	< 4.7
4	0	-24	19.9	19.4
4	0	-22	-66.7	75.5
4	0	-20	-1.3	< 4.7
4	0	-18	67.4	73.1
4	0	-16	-32.2	28.8
4	0	-14	37.2	33.7
4	0	-12	-18.3	20.6
4	0	-10	-187.3	182.6
4	0	-8	2.8	6.3
4	0	-6	-42.3	41.8
4	0	-4	-118.8	124.4
4	0	-2	72.2	87.2
4	0	0	-10.9	11.3
4	0	2	-37.8	44.2
4	0	4	14.5	20.8
4	0	6	-89.2	84.9
4	0	8	-21.9	20.9
4	0	10	26.4	24.2
4	0	12	-43.7	45.0
4	0	14	11.6	12.7
4	0	16	25.4	21.3
4	0	18	-22.4	20.2
4	0	20	7.3	9.4
4	0	22	11.5	8.7
4	0	24	-3.2	< 3.7
4	0	26	9.5	< 2.7
6	0	-30	-14.4	13.5
6	0	-28	18.1	16.1
6	0	-26	-4.9	< 4.7
6	0	-24	-30.1	27.5
6	0	-22	15.0	11.4
6	0	-20	-22.5	20.8
6	0	-18	-17.9	18.7
6	0	-16	29.0	27.7
6	0	-14	-64.9	64.0
6	0	-12	-30.3	27.6
6	0	-10	46.5	46.8
6	0	-8	-7.0	12.3
6	0	-6	57.7	61.8
6	0	-4	-28.9	33.5
6	0	-2	-27.0	31.0
6	0	0	133.6	134.7
6	0	2	-32.0	37.4
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6	0	6	78.7	78.5
6	0	8	-21.4	19.9
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6	0	12	46.8	43.4
6	0	14	-36.0	35.1
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6	0	18	19.0	18.7
6	0	20	-9.8	< 4.3
6	0	22	12.9	10.1
6	0	24	2.2	< 2.5
8	0	-30	-2.3	< 3.6
8	0	-28	-14.3	12.7
8	0	-26	20.9	17.2
8	0	-24	-6.5	< 4.9
8	0	-22	-5.2	< 4.9
8	0	-20	32.9	29.4
8	0	-18	-7.6	< 4.6
8	0	-16	21.6	22.1
8	0	-14	26.8	25.3
8	0	-12	39.8	39.8
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8	0	-6	-22.5	24.6
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8	0	22	-3.9	< 1.9
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10	0	-16	-10.6	9.2
10	0	-14	30.3	30.4
10	0	-12	10.9	10.6
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10	0	8	-6.9	< 4.9
10	0	10	-4.7	< 4.9
10	0	12	-35.0	32.4
10	0	14	-3.5	< 4.2
10	0	16	10.9	7.1
10	0	18	-2.5	< 2.7
12	0	-30	-14.3	13.3
12	0	-28	14.5	10.1
12	0	-26	-3.5	< 4.2
12	0	-24	-19.7	15.5
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16	0	-8	12.0	15.8
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16	0	-4	-11.4	15.0
16	0	-2	11.5	10.0
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18	0	-18	-3.4	< 2.7
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1	1	-27	6.7	8.4
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1	1	-22	-1.3	5.5
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1	1	-16	34.1	35.5
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1	1	7	21.2	19.9
1	1	8	15.4	13.1
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1	1	10	-70.7	65.0
1	1	11	29.6	28.2
1	1	12	-13.4	14.4
1	1	13	-42.2	40.7
1	1	14	-7.7	9.0
1	1	15	-24.8	25.4
1	1	16	-12.6	11.8
1	1	17	12.4	12.2
1	1	18	-0.5	< 2.6
1	1	19	-30.3	28.9
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1	1	21	1.5	< 2.7
1	1	22	10.6	10.4
1	1	23	8.7	9.1
1	1	24	5.4	5.5
1	1	25	-11.9	10.6
1	1	26	-11.5	11.8
1	1	27	8.6	9.0
3	1	-29	-2.1	< 1.9
3	1	-28	-3.5	6.1
3	1	-27	9.6	10.3
3	1	-26	0.0	4.5
3	1	-25	-20.0	22.8
3	1	-24	-4.6	4.9
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3	1	-22	17.0	18.4
3	1	-21	10.3	9.0
3	1	-20	42.8	45.0
3	1	-19	-17.3	18.9
3	1	-18	-11.3	9.3
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3	1	-15	25.5	24.4
3	1	-14	0.8	< 2.0
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3	1	-11	-14.9	13.6
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3	1	-9	-7.8	10.8
3	1	-8	32.3	35.3
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3	1	-6	-16.3	13.9
3	1	-5	12.7	15.0
3	1	-4	27.6	28.4
3	1	-3	2.2	4.1
3	1	-2	-2.0	4.1
3	1	-1	-54.0	53.0
3	1	0	-63.1	61.8
3	1	1	22.9	22.8
3	1	2	-17.3	16.6
3	1	3	-7.0	7.8
3	1	4	-43.4	38.5
3	1	5	-18.1	19.8
3	1	6	-53.4	45.3
3	1	7	46.6	42.0
3	1	8	-5.8	5.7
3	1	9	-23.7	22.1
3	1	10	-19.0	15.9
3	1	11	-20.6	20.2
3	1	12	6.0	8.2
3	1	13	26.7	26.2
3	1	14	27.9	27.7
3	1	15	-14.4	11.2
3	1	16	-21.6	17.7
3	1	17	3.4	5.4
3	1	18	-10.1	9.3
3	1	19	22.9	20.9
3	1	20	17.3	12.1
3	1	21	-7.0	6.4
3	1	22	-7.0	8.8
3	1	23	8.4	8.2
3	1	24	-4.1	4.8
3	1	25	10.7	11.3
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5	1	-18	-4.2	< 2.5
5	1	-17	-25.9	25.1
5	1	-16	-7.8	5.2
5	1	-15	-43.2	42.2
5	1	-14	-20.7	25.0
5	1	-13	35.3	33.8
5	1	-12	58.1	56.4
5	1	-11	-30.3	31.1
5	1	-10	-4.8	7.5
5	1	-9	30.9	32.9
5	1	-8	-67.1	71.6
5	1	-7	77.3	76.8
5	1	-6	-18.1	18.1
5	1	-5	-24.7	25.7
5	1	-4	-20.7	19.7
5	1	-3	67.7	67.0
5	1	-2	7.1	5.7
5	1	-1	31.8	35.3
5	1	0	-4.5	6.7
5	1	1	-35.5	35.7
5	1	2	-9.2	11.7
5	1	3	49.9	47.6
5	1	4	54.8	50.3
5	1	5	1.9	4.0
5	1	6	11.0	12.8
5	1	7	-2.7	5.1
5	1	8	-17.4	16.0
5	1	9	50.6	45.7
5	1	10	15.5	17.3
5	1	11	-11.5	10.4
5	1	12	-11.0	11.6
5	1	13	-3.6	5.9
5	1	14	-3.5	4.9
5	1	15	26.7	24.2
5	1	16	9.7	9.8
5	1	17	-8.2	8.6
5	1	18	1.0	< 2.6
5	1	19	4.8	5.8
5	1	20	2.9	< 2.4
5	1	21	10.3	10.5
5	1	22	3.6	5.5
5	1	23	-9.5	10.2
5	1	24	-5.6	5.6
7	1	-30	-9.9	9.9
7	1	-29	10.1	8.9
7	1	-28	-1.6	4.1
7	1	-27	4.3	4.8
7	1	-26	4.8	5.7
7	1	-25	-11.4	10.3
7	1	-24	-5.3	< 2.7
7	1	-23	17.3	15.4
7	1	-22	6.3	6.1
7	1	-21	4.8	6.6
7	1	-20	0.5	< 2.6
7	1	-19	-5.6	4.8
7	1	-18	-17.0	17.8
7	1	-17	28.3	26.8
7	1	-16	1.4	< 2.4
7	1	-15	-7.3	7.2
7	1	-14	-1.4	< 2.2
7	1	-13	5.8	5.7
7	1	-12	5.9	6.2
7	1	-11	54.0	49.6
7	1	-10	20.4	20.0
7	1	-9	-10.6	8.3
7	1	-8	-12.0	8.5
7	1	-7	17.5	17.7
7	1	-6	44.1	39.3
7	1	-5	46.3	44.0
7	1	-4	56.5	47.7
7	1	-3	-49.7	46.8
7	1	-2	-50.7	51.9
7	1	-1	10.8	13.3
7	1	0	-6.2	< 2.0
7	1	1	-0.6	< 2.0
7	1	2	37.6	36.9
7	1	3	-60.8	58.6
7	1	4	-13.5	15.9
7	1	5	45.3	42.2
7	1	6	34.6	32.4
7	1	7	16.5	17.4
7	1	8	14.9	11.5
7	1	9	-30.2	29.9
7	1	10	-30.2	32.7
7	1	11	16.7	15.0
7	1	12	17.9	16.5
7	1	13	-16.1	15.0
7	1	14	10.6	10.2
7	1	15	-17.7	19.2
7	1	16	11.0	10.8
7	1	17	14.1	14.6
7	1	18	2.6	< 2.3
7	1	19	-10.0	10.8
7	1	20	5.0	7.2
7	1	21	-5.2	6.6
9	1	-31	4.1	4.2
9	1	-30	12.6	12.1
9	1	-29	-12.0	10.8
9	1	-28	-1.6	< 2.1
9	1	-27	9.1	9.4
9	1	-26	-3.8	7.0
9	1	-25	-0.3	< 2.5
9	1	-24	3.4	< 2.6
9	1	-23	-14.8	13.8
9	1	-22	0.4	< 2.7
9	1	-21	20.8	20.2
9	1	-20	19.2	18.4
9	1	-19	-2.7	4.9
9	1	-18	6.7	9.2
9	1	-17	-8.6	7.6
9	1	-16	-0.2	4.7
9	1	-15	16.7	16.5
9	1	-14	23.4	22.1
9	1	-13	34.4	34.4
9	1	-12	-4.6	4.4
9	1	-11	-9.0	8.2
9	1	-10	-5.8	6.4
9	1	-9	14.7	14.2
9	1	-8	7.3	7.3
9	1	-7	-41.5	36.2
9	1	-6	-23.6	24.0
9	1	-5	-8.8	11.2
9	1	-4	-1.3	4.2
9	1	-3	2.0	< 2.2
9	1	-2	17.4	21.0
9	1	-1	-36.2	43.2
9	1	0	2.6	< 2.3
9	1	1	7.8	8.8
9	1	2	14.5	13.9
9	1	3	13.9	15.9
9	1	4	5.0	5.1
9	1	5	-14.1	17.1
9	1	6	-25.5	24.9
9	1	7	3.0	< 2.6
9	1	8	-23.0	20.6
9	1	9	-17.1	18.5
9	1	10	-8.6	8.2
9	1	11	-22.4	21.4
9	1	12	7.2	7.9
9	1	13	6.3	7.7
9	1	14	9.1	9.9
9	1	15	3.5	4.3
9	1	16	-4.9	5.8
9	1	17	2.6	< 1.9
9	1	18	-2.6	4.6
9	1	19	6.1	6.7
11	1	-30	6.1	5.6
11	1	-29	2.4	< 1.7
11	1	-28	3.1	4.9
11	1	-27	-14.3	12.8
11	1	-26	-9.2	5.7
11	1	-25	9.6	8.6
11	1	-24	14.9	13.7
11	1	-23	-2.3	< 2.6
11	1	-22	8.3	8.4
11	1	-21	-14.9	13.6
11	1	-20	-23.2	21.5
11	1	-19	22.9	20.5
11	1	-18	-1.4	< 2.7
11	1	-17	-28.3	24.7
11	1	-16	-22.6	20.5
11	1	-15	-40.6	37.4
11	1	-14	-17.0	16.1
11	1	-13	23.4	19.0
11	1	-12	48.9	40.6
11	1	-11	-17.0	16.8
11	1	-10	-1.4	< 2.6
11	1	-9	7.3	7.2
11	1	-8	-25.1	25.3
11	1	-7	39.3	38.7
11	1	-6	16.0	16.6
11	1	-5	-31.2	32.2
11	1	-4	-20.4	19.3
11	1	-3	1.4	< 2.6
11	1	-2	-14.1	15.6
11	1	-1	16.2	18.4
11	1	0	3.0	< 2.6
11	1	1	-26.5	27.5
11	1	2	22.6	22.6
11	1	3	13.1	14.1
11	1	4	2.4	6.3
11	1	5	6.1	8.0
11	1	6	8.1	8.7
11	1	7	-13.2	13.4
11	1	8	-3.6	4.8
11	1	9	16.8	18.3
11	1	10	13.8	15.7
11	1	11	3.4	5.2
11	1	12	1.2	< 2.2
11	1	13	0.2	< 2.0
11	1	14	-8.0	9.1
11	1	15	11.8	12.9
11	1	16	0.9	3.2
13	1	-28	-5.1	6.4
13	1	-27	3.5	< 1.8
13	1	-26	1.1	< 2.0
13	1	-25	-12.4	9.7
13	1	-24	-9.0	8.3
13	1	-23	8.4	5.8
13	1	-22	-0.1	< 2.4
13	1	-21	5.0	5.0
13	1	-20	5.5	6.0
13	1	-19	-14.7	12.8
13	1	-18	-9.4	8.5
13	1	-17	12.0	11.3
13	1	-16	8.2	7.8
13	1	-15	8.2	9.6
13	1	-14	18.0	20.2
13	1	-13	4.1	5.9
13	1	-12	10.5	12.0
13	1	-11	33.4	38.0
13	1	-10	22.3	24.4
13	1	-9	-1.2	< 2.7
13	1	-8	-19.2	19.8
13	1	-7	-18.6	20.2
13	1	-6	0.4	< 2.7
13	1	-5	5.1	9.4
13	1	-4	20.2	23.1
13	1	-3	-8.2	10.0
13	1	-2	9.9	10.0
13	1	-1	10.5	13.6
13	1	0	6.4	9.2
13	1	1	19.3	22.9
13	1	2	3.8	5.4
13	1	3	-5.4	8.2
13	1	4	-4.6	6.3
13	1	5	9.7	11.9
13	1	6	4.6	8.2
13	1	7	4.2	5.5
13	1	8	-2.3	< 2.1
13	1	9	-10.4	12.7
13	1	10	-8.5	10.5
13	1	11	3.8	5.0
13	1	12	5.8	7.4
15	1	-27	9.4	10.7
15	1	-26	4.1	6.8
15	1	-25	9.9	10.3
15	1	-24	5.9	6.9
15	1	-23	5.9	5.6
15	1	-22	-10.6	11.7
15	1	-21	15.2	16.2
15	1	-20	2.2	3.6
15	1	-19	0.7	< 2.3
15	1	-18	-0.9	< 2.3
15	1	-17	-10.7	10.0
15	1	-16	-8.0	9.4
15	1	-15	12.0	13.5
15	1	-14	12.6	14.8
15	1	-13	-7.5	8.9
15	1	-12	1.4	4.1
15	1	-11	-5.1	4.2
15	1	-10	1.1	4.1
15	1	-9	10.1	12.2
15	1	-8	16.7	16.0
15	1	-7	-12.2	14.3
15	1	-6	0.2	4.1
15	1	-5	2.4	< 2.4
15	1	-4	2.0	< 2.4
15	1	-3	13.7	15.4
15	1	-2	1.8	5.5
15	1	-1	-8.5	9.7
15	1	0	-15.5	16.1
15	1	1	0.9	< 2.1
15	1	2	-0.3	< 2.0
15	1	3	-0.1	3.2
15	1	4	8.8	9.9
15	1	5	-11.9	12.1
15	1	6	-3.1	5.2
17	1	-22	6.5	6.8
17	1	-21	-14.1	14.8
17	1	-20	4.9	7.0
17	1	-19	2.0	< 1.6
17	1	-18	5.6	5.6
17	1	-17	-1.7	< 1.8
17	1	-16	-0.6	< 1.9

Table 8 (*cont.*)

h	k	l	F(calc)	F(meas)
17	1	-15	-9.0	11.4
17	1	-14	-3.1	< 1.9
17	1	-13	11.3	11.2
17	1	-12	6.7	8.0
17	1	-11	-1.9	< 2.0
17	1	-10	-7.5	10.2
17	1	-9	-5.3	7.6
17	1	-8	-9.8	12.4
17	1	-7	6.0	6.9
17	1	-6	5.2	6.7
17	1	-5	-11.5	13.6
17	1	-4	-2.2	3.1
17	1	-3	-3.4	4.0
17	1	-2	0.3	< 1.5
17	1	-1	6.2	8.6
0	2	2	12.3	16.8
0	2	3	68.9	63.1
0	2	4	-24.4	25.5
0	2	5	74.4	72.3
0	2	6	-25.5	25.4
0	2	7	-90.2	86.8
0	2	8	12.4	12.8
0	2	9	-5.7	8.1
0	2	10	-13.0	12.4
0	2	11	-0.7	3.1
0	2	12	-16.9	14.5
0	2	13	-45.1	42.4
0	2	14	7.8	7.2
0	2	15	11.3	11.8
0	2	16	-10.3	8.9
0	2	17	-12.3	11.4
0	2	18	-2.8	< 2.7
0	2	19	-13.6	10.0
0	2	20	13.2	12.9
0	2	21	13.7	14.0
0	2	22	-8.8	7.8
0	2	23	-9.7	10.3
0	2	24	-5.7	6.2
2	2	-26	-5.9	6.0
2	2	-25	-3.3	4.2
2	2	-24	8.4	8.9
2	2	-23	12.5	12.3
2	2	-22	-3.7	6.0
2	2	-21	15.3	16.0
2	2	-20	-14.3	14.7
2	2	-19	-8.7	6.2
2	2	-18	6.0	5.4
2	2	-17	2.4	4.9
2	2	-16	-6.4	9.2
2	2	-15	-12.0	10.5
2	2	-14	-7.3	6.2
2	2	-13	-32.6	35.5
2	2	-12	17.2	17.4
2	2	-11	7.3	6.0
2	2	-10	-1.3	< 1.9
2	2	-9	-13.3	13.1
2	2	-8	9.0	13.4
2	2	-7	-36.3	35.3
2	2	-6	10.8	10.8
2	2	-5	8.4	9.8
2	2	-4	-31.2	32.0
2	2	-3	-23.6	25.4
2	2	-2	-4.8	4.4
2	2	-1	-24.7	24.2
2	2	0	5.5	3.6
2	2	1	30.3	29.2
2	2	2	-44.6	39.4
2	2	3	-30.0	27.9
2	2	4	19.2	17.8
2	2	5	-52.7	48.9
2	2	6	33.9	31.8
2	2	7	-24.0	23.1
2	2	8	-8.8	6.5
2	2	9	-23.3	20.0
2	2	10	21.5	20.7
2	2	11	21.9	22.0
2	2	12	-1.6	< 2.5
2	2	13	7.9	11.2
2	2	14	-26.8	24.2
2	2	15	-13.8	11.7
2	2	16	14.8	11.8
2	2	17	18.5	15.3
2	2	18	10.8	9.4
2	2	19	-3.0	5.7
2	2	20	-8.0	8.4
2	2	21	-5.7	7.2
2	2	22	6.3	7.1
2	2	23	11.3	10.4
2	2	24	1.2	< 1.9
2	2	25	-9.1	8.9
4	2	-29	-12.5	11.6
4	2	-28	1.2	< 1.8
4	2	-27	4.7	6.5
4	2	-26	4.6	5.0
4	2	-25	13.9	16.2
4	2	-24	-2.3	< 2.5
4	2	-23	-20.6	19.7
4	2	-22	4.0	< 2.7
4	2	-21	1.3	< 2.7
4	2	-20	5.1	6.6
4	2	-19	-19.2	19.2
4	2	-18	11.2	11.3
4	2	-17	-50.6	49.1
4	2	-16	15.8	14.2
4	2	-15	37.9	34.2
4	2	-14	-11.2	11.3
4	2	-13	16.3	14.6
4	2	-12	-11.8	14.0
4	2	-11	-28.7	28.9
4	2	-10	4.0	3.7
4	2	-9	34.2	33.6
4	2	-8	-7.7	7.6
4	2	-7	-22.8	21.2
4	2	-6	23.8	25.6
4	2	-5	-24.9	23.4
4	2	-4	22.4	21.9
4	2	-3	29.9	29.1
4	2	-2	-9.8	10.1
4	2	-1	-24.2	26.9
4	2	0	25.2	25.6
4	2	1	16.1	18.5
4	2	2	18.9	20.0
4	2	3	40.5	34.3
4	2	4	-19.5	16.8
4	2	5	-15.5	14.9
4	2	6	1.4	< 2.1
4	2	7	25.9	24.4
4	2	8	2.7	4.7
4	2	9	18.6	15.9
4	2	10	-13.2	12.3
4	2	11	-11.1	10.2
4	2	12	10.5	8.7
4	2	13	24.2	21.2
4	2	14	12.3	11.3
4	2	15	7.0	6.2
4	2	16	5.4	5.0
4	2	17	-7.6	9.0
4	2	18	6.6	5.9
4	2	19	12.3	11.9
4	2	20	-5.7	4.7
4	2	21	-3.5	4.4
4	2	22	-5.3	6.3
4	2	23	-7.1	6.6
6	2	-29	-6.5	5.6
6	2	-28	-0.9	< 1.8
6	2	-27	-6.5	5.6
6	2	-26	7.6	7.6
6	2	-25	-3.7	6.0
6	2	-24	-1.4	< 2.5
6	2	-23	16.7	16.4
6	2	-22	-11.9	10.7
6	2	-21	-16.5	16.0
6	2	-20	10.2	8.0
6	2	-19	-0.1	5.5
6	2	-18	-6.4	7.9
6	2	-17	33.6	31.6
6	2	-16	-15.5	14.5
6	2	-15	-1.4	< 2.5
6	2	-14	20.0	19.7
6	2	-13	16.4	16.2
6	2	-12	-1.0	< 2.3
6	2	-11	3.4	5.6
6	2	-10	5.4	8.4
6	2	-9	-18.0	16.1
6	2	-8	48.3	47.1
6	2	-7	40.7	39.8
6	2	-6	-26.5	26.4
6	2	-5	-1.1	4.6
6	2	-4	-46.7	44.2
6	2	-3	-0.9	4.6
6	2	-2	10.0	12.5
6	2	-1	39.3	41.0
6	2	0	-16.5	14.6
6	2	1	-15.7	16.7
6	2	2	1.3	6.2
6	2	3	28.8	26.9
6	2	4	21.8	21.8
6	2	5	28.4	25.8
6	2	6	-7.3	8.3
6	2	7	-43.4	40.4
6	2	8	4.7	< 2.6
6	2	9	12.0	9.8
6	2	10	7.9	10.0
6	2	11	12.6	11.5
6	2	12	-13.2	11.6
6	2	13	-20.9	19.2
6	2	14	-2.6	5.5
6	2	15	11.6	11.1
6	2	16	-4.4	5.1
6	2	17	-4.0	5.7
6	2	18	-7.5	8.9
6	2	19	-12.5	13.0
6	2	20	4.3	4.6
6	2	21	8.2	8.8
8	2	-28	-6.3	7.7
8	2	-27	14.1	11.3
8	2	-26	-7.8	7.1
8	2	-25	-4.2	< 2.4
8	2	-24	6.4	7.1
8	2	-23	5.5	8.3
8	2	-22	3.3	5.6
8	2	-21	12.4	10.0
8	2	-20	-5.0	5.1
8	2	-19	-11.7	8.8
8	2	-18	9.2	8.8
8	2	-17	11.7	11.2
8	2	-16	-3.1	< 2.7
8	2	-15	8.4	7.7
8	2	-14	-17.6	15.9
8	2	-13	-14.9	12.7
8	2	-12	-0.4	< 2.5
8	2	-11	16.0	12.9
8	2	-10	-6.5	6.7
8	2	-9	-6.8	7.7
8	2	-8	-15.6	16.9
8	2	-7	-22.0	19.5
8	2	-6	0.0	< 2.3
8	2	-5	21.0	20.4
8	2	-4	0.1	< 2.4
8	2	-3	-10.6	10.1
8	2	-2	9.1	7.7
8	2	-1	-12.1	14.2
8	2	0	16.3	17.3
8	2	1	29.8	29.8
8	2	2	-14.4	11.7
8	2	3	-25.1	26.3
8	2	4	-11.0	13.3
8	2	5	-38.8	37.3
8	2	6	-7.2	7.7
8	2	7	-0.1	< 2.7
8	2	8	-11.7	10.1
8	2	9	-11.3	10.8
8	2	10	7.0	5.5
8	2	11	5.8	9.3
8	2	12	1.9	< 2.6
8	2	13	13.2	14.0
8	2	14	-6.6	6.9
8	2	15	-10.6	13.6
8	2	16	8.9	8.9
8	2	17	-2.5	< 1.9
8	2	18	2.9	3.7
10	2	-28	4.5	5.2
10	2	-27	-4.8	< 1.8
10	2	-26	11.4	10.9
10	2	-25	7.4	8.7
10	2	-24	-7.8	8.6
10	2	-23	-10.5	11.1
10	2	-22	-1.4	4.7
10	2	-21	-2.4	4.8
10	2	-20	-2.2	4.9
10	2	-19	-8.6	10.6
10	2	-18	-14.0	14.3
10	2	-17	-25.6	23.8
10	2	-16	10.5	10.1
10	2	-15	22.8	23.7
10	2	-14	9.6	10.8
10	2	-13	3.7	5.0
10	2	-12	-4.0	6.5
10	2	-11	-25.6	21.5
10	2	-10	14.2	11.9
10	2	-9	15.1	12.7
10	2	-8	1.7	< 2.6
10	2	-7	-18.6	19.0
10	2	-6	-8.5	9.8
10	2	-5	-19.2	19.0
10	2	-4	1.4	< 2.6
10	2	-3	18.3	18.5
10	2	-2	-10.7	9.9
10	2	-1	-20.1	21.7
10	2	0	-1.7	< 2.7
10	2	1	-9.6	8.2
10	2	2	11.4	13.1
10	2	3	10.3	10.9
10	2	4	-3.4	5.1
10	2	5	-11.0	10.1
10	2	6	6.6	6.1
10	2	7	14.1	14.8
10	2	8	11.6	12.5
10	2	9	14.8	13.7
10	2	10	-6.4	6.9
10	2	11	-5.7	7.0
10	2	12	-0.7	< 2.2
10	2	13	1.6	< 2.0
10	2	14	4.0	6.3
10	2	15	-6.2	6.9
12	2	-27	-8.2	7.2
12	2	-26	2.0	< 1.7
12	2	-25	-4.6	6.2
12	2	-24	2.6	3.8
12	2	-23	10.2	7.4
12	2	-22	-3.8	< 2.3
12	2	-21	-18.3	14.1
12	2	-20	5.7	< 2.5
12	2	-19	0.6	< 2.5
12	2	-18	6.8	8.3
12	2	-17	29.6	25.9
12	2	-16	-1.1	< 2.7
12	2	-15	-9.8	9.1
12	2	-14	2.5	< 2.7
12	2	-13	-8.8	< 2.7
12	2	-12	-8.3	8.8
12	2	-11	-2.8	5.1
12	2	-10	-3.2	< 2.8
12	2	-9	-32.6	29.0
12	2	-8	16.6	16.1
12	2	-7	18.0	20.9
12	2	-6	-5.1	5.1
12	2	-5	23.1	26.2
12	2	-4	-4.7	7.5
12	2	-3	-2.5	< 2.7
12	2	-2	15.0	16.5
12	2	-1	17.0	20.7
12	2	0	-2.9	< 2.7
12	2	1	-0.3	< 2.6
12	2	2	-0.2	< 2.6
12	2	3	-3.3	< 2.5
12	2	4	6.3	8.9
12	2	5	10.4	10.9
12	2	6	-9.5	9.1
12	2	7	-8.8	11.6
12	2	8	-1.2	< 2.1
12	2	9	0.6	< 1.9
12	2	10	6.2	8.8
12	2	11	5.7	7.1
14	2	-21	7.3	5.0
14	2	-20	-5.8	5.8
14	2	-19	-5.3	4.5
14	2	-18	3.8	5.0
14	2	-17	5.3	6.4
14	2	-16	3.5	6.5
14	2	-15	3.9	5.3
14	2	-14	-7.2	6.8
14	2	-13	-9.4	6.2
14	2	-12	6.1	6.8
14	2	-11	7.9	8.9
14	2	-10	4.8	5.7
14	2	-9	9.5	8.1
14	2	-8	-11.0	12.8
14	2	-7	8.2	6.5
14	2	-6	-0.8	< 2.5
14	2	-5	11.2	10.8
14	2	-4	-1.1	< 2.5
14	2	-3	-12.5	12.2
14	2	-2	-4.5	7.5
14	2	-1	-11.1	11.7
14	2	0	8.8	10.7
14	2	1	5.2	8.4
14	2	2	-0.1	< 2.1
14	2	3	-5.1	6.9
14	2	4	-7.2	10.1
16	2	-19	10.5	7.6
16	2	-18	-8.0	7.2
16	2	-17	-5.8	4.8
16	2	-16	3.6	3.1
16	2	-15	3.0	3.5
16	2	-14	1.5	< 1.4
16	2	-13	2.9	< 1.5
16	2	-12	-6.6	8.0
16	2	-11	-13.3	12.1
16	2	-10	3.5	2.5
16	2	-9	3.1	3.0
16	2	-8	1.6	2.7
16	2	-7	-2.5	2.7
16	2	-6	-2.8	3.5
16	2	-5	-9.5	7.3
16	2	-4	3.8	3.7
16	2	-3	5.9	6.3
16	2	-2	-0.7	< 1.3
16	2	-1	-3.4	4.6
1	3	-24	6.1	5.8
1	3	-23	0.6	< 1.6
1	3	-22	-7.6	6.0
1	3	-21	3.1	5.2
1	3	-20	-3.2	4.8
1	3	-19	-3.0	4.1
1	3	-18	5.6	6.4
1	3	-17	0.6	< 2.2
1	3	-16	-15.5	14.5
1	3	-15	2.0	< 2.2
1	3	-14	2.1	< 2.2
1	3	-13	2.3	< 2.2
1	3	-12	6.4	7.2
1	3	-11	9.1	9.2
1	3	-10	-27.2	24.9
1	3	-9	-8.9	8.7
1	3	-8	-0.5	3.8
1	3	-7	-1.9	3.8
1	3	-6	-6.2	6.0
1	3	-5	17.3	19.2
1	3	-4	-23.9	20.3
1	3	-3	-5.1	3.8
1	3	3	-25.2	23.1
1	3	4	20.5	16.5
1	3	5	2.9	4.6
1	3	6	-30.2	26.4
1	3	7	24.8	22.8
1	3	8	-10.0	8.2
1	3	9	-1.9	3.5
1	3	10	22.3	19.7
1	3	11	-13.4	12.9
1	3	12	-15.2	12.5
1	3	13	-1.3	3.9
1	3	14	10.9	11.4
1	3	15	5.7	5.6
1	3	16	12.2	10.4
1	3	17	-3.4	3.8
1	3	18	-14.6	12.3
1	3	19	0.1	< 2.0
1	3	20	8.9	7.3
1	3	21	3.8	4.1
1	3	22	4.1	4.1
1	3	23	-4.0	3.1
3	3	-24	-1.4	< 1.5
3	3	-23	-2.6	4.5
3	3	-22	4.3	4.1
3	3	-21	-0.8	< 2.0
3	3	-20	-14.0	15.2
3	3	-19	3.3	4.4
3	3	-18	-2.1	4.5
3	3	-17	11.4	15.1
3	3	-16	4.2	< 2.2
3	3	-15	0.6	< 2.2
3	3	-14	-9.2	8.7
3	3	-13	-12.3	15.5
3	3	-12	15.1	11.9
3	3	-11	-4.0	4.4
3	3	-10	6.7	7.6
3	3	-9	-2.2	3.3
3	3	-8	-9.0	7.7
3	3	-7	-4.7	6.3
3	3	-6	20.4	20.3
3	3	-5	-0.5	2.9
3	3	-4	3.4	3.6
3	3	-3	-1.6	< 1.4
3	3	-2	-4.5	3.9
3	3	-1	3.9	4.8
3	3	0	21.3	16.9
3	3	1	0.3	2.1
3	3	2	-8.6	9.1
3	3	3	-2.4	3.4
3	3	4	-7.5	7.4
3	3	5	12.9	12.5
3	3	6	20.5	16.9
3	3	7	-1.7	< 2.0
3	3	8	1.6	3.7
3	3	9	-11.9	10.9
3	3	10	11.6	10.0
3	3	11	9.0	7.6
3	3	12	20.8	16.2
3	3	13	7.3	6.1
3	3	14	-6.1	6.1
3	3	15	-0.8	< 2.2
3	3	16	-1.9	3.7
3	3	17	5.4	6.5
3	3	18	1.4	< 1.9
3	3	19	-2.5	< 1.7
3	3	20	-6.3	6.2
3	3	21	-4.5	5.2
5	3	-26	7.0	4.7
5	3	-25	-0.3	< 1.4
5	3	-24	-7.4	7.1
5	3	-23	1.7	< 1.8
5	3	-22	-1.4	4.2
5	3	-21	-5.5	5.3
5	3	-20	15.1	13.4
5	3	-19	7.9	9.5
5	3	-18	-6.0	4.8
5	3	-17	-3.6	4.9
5	3	-16	18.9	17.1
5	3	-15	-23.6	19.8
5	3	-14	22.5	21.1
5	3	-13	3.4	5.2
5	3	-12	-19.2	15.4
5	3	-11	15.4	13.1
5	3	-10	10.8	9.6
5	3	-9	1.5	< 2.0
5	3	-8	-5.0	8.4
5	3	-7	-0.7	4.7
5	3	-6	-25.7	25.5
5	3	-5	-0.4	< 1.3
5	3	-4	31.1	26.6
5	3	-3	-3.4	< 1.8
5	3	-2	5.0	6.0
5	3	-1	0.7	< 1.8
5	3	0	-4.1	6.2
5	3	1	10.6	10.3
5	3	2	27.9	25.1
5	3	3	1.6	< 2.0
5	3	4	-11.3	10.2
5	3	5	-7.1	9.1
5	3	6	-6.7	6.0
5	3	7	9.9	9.8
5	3	8	11.3	9.9
5	3	9	5.1	6.1
5	3	10	-17.4	14.7
5	3	11	-7.4	8.4
5	3	12	-2.6	4.7
5	3	13	1.4	< 2.1
5	3	14	2.0	< 2.1
5	3	15	-3.1	< 2.0
5	3	16	-11.3	10.6
5	3	17	-4.1	5.8
5	3	18	5.4	6.0
5	3	19	3.4	4.6
7	3	-24	9.1	7.7
7	3	-23	-0.8	< 1.7
7	3	-22	-3.8	< 1.9
7	3	-21	5.6	6.1
7	3	-20	-4.4	3.7
7	3	-19	2.1	3.8
7	3	-18	8.2	6.7
7	3	-17	-4.5	5.6
7	3	-16	-13.7	12.6
7	3	-15	3.7	< 2.2
7	3	-14	-7.0	7.4
7	3	-13	8.9	8.8
7	3	-12	6.0	5.2
7	3	-11	-2.3	3.5
7	3	-10	-19.7	17.5
7	3	-9	-5.6	5.4
7	3	-8	6.0	5.3
7	3	-7	2.9	4.6
7	3	-6	17.7	16.9
7	3	-5	-2.8	3.7
7	3	-4	-11.3	9.5
7	3	-3	4.1	4.4
7	3	-2	5.7	5.9
7	3	-1	13.4	13.3
7	3	0	-13.3	10.6
7	3	1	-11.9	14.2
7	3	2	-29.2	28.1
7	3	3	-17.6	17.0
7	3	4	3.8	< 2.2
7	3	5	7.6	9.4
7	3	6	-9.4	7.4
7	3	7	2.6	3.9
7	3	8	-3.6	3.9
7	3	9	-3.7	3.8
7	3	10	15.8	13.9
7	3	11	1.2	< 2.0
7	3	12	-6.7	6.0
7	3	13	-4.0	6.3
7	3	14	-0.6	< 1.7
7	3	15	-0.4	< 1.5
7	3	16	4.1	3.9
9	3	-24	-10.1	8.4
9	3	-23	-1.0	< 1.6
9	3	-22	4.1	< 1.7
9	3	-21	-3.9	3.8
9	3	-20	-10.1	9.0
9	3	-19	2.2	3.6
9	3	-18	1.6	3.7
9	3	-17	4.5	6.6
9	3	-16	11.7	9.5
9	3	-15	-1.3	3.5
9	3	-14	10.4	7.9
9	3	-13	-2.7	3.9
9	3	-12	2.1	< 2.2
9	3	-11	3.3	3.9
9	3	-10	-0.1	< 2.2
9	3	-9	-1.0	< 2.2
9	3	-8	-16.4	14.0
9	3	-7	-3.8	4.8
9	3	-6	5.8	4.8
9	3	-5	1.2	< 2.2
9	3	-4	-2.2	3.9
9	3	-3	-4.6	4.9
9	3	-2	-11.6	9.8
9	3	-1	4.7	4.0
9	3	0	10.7	9.4
9	3	1	-1.8	< 2.2
9	3	2	0.6	< 2.2
9	3	3	3.6	< 2.2
9	3	4	0.2	< 2.2
9	3	5	10.5	10.4
9	3	6	15.4	14.2
9	3	7	-0.8	< 2.0
9	3	8	-1.6	< 2.0
9	3	9	-6.6	7.5
9	3	10	-3.8	4.1
11	3	-23	-5.4	5.2
11	3	-22	-1.2	3.8
11	3	-21	2.5	4.7
11	3	-20	13.2	11.9
11	3	-19	9.0	10.4
11	3	-18	-4.3	< 1.9
11	3	-17	-7.0	8.5
11	3	-16	-1.5	4.8
11	3	-15	-9.6	9.3
11	3	-14	6.8	5.7
11	3	-13	1.4	< 2.1
11	3	-12	-14.1	11.7
11	3	-11	-2.6	< 2.2
11	3	-10	6.6	5.2
11	3	-9	4.1	8.2
11	3	-8	11.6	11.9
11	3	-7	6.2	6.7
11	3	-6	-5.1	4.7
11	3	-5	-5.7	7.0
11	3	-4	17.2	16.6
11	3	-3	0.9	2.9
11	3	-2	3.4	3.7
11	3	-1	3.8	2.9
11	3	0	-12.1	10.4
11	3	1	0.5	< 2.0
11	3	2	10.6	9.9
11	3	3	1.3	< 1.9
11	3	4	-2.2	3.6
11	3	5	-3.5	6.0
11	3	6	-4.0	4.2
11	3	7	0.1	2.7
11	3	8	8.5	10.4
11	3	9	2.7	4.9
13	3	-19	-2.6	< 1.4
13	3	-18	7.4	5.6
13	3	-17	-4.7	5.4
13	3	-16	-5.7	5.1
13	3	-15	3.2	3.7
13	3	-14	-2.5	< 1.8
13	3	-13	5.2	6.1
13	3	-12	9.5	0.9
13	3	-11	3.2	3.6
13	3	-10	-5.3	4.4
13	3	-9	2.9	3.6
13	3	-8	3.5	4.9
13	3	-7	-6.1	5.7
13	3	-6	9.3	8.4
13	3	-5	-9.0	11.2
13	3	-4	-10.5	11.7
13	3	-3	5.5	5.3
13	3	-2	-1.8	< 1.7
13	3	-1	6.5	8.9
13	3	0	0.3	< 1.5
13	3	1	-3.9	5.9
13	3	2	-7.3	9.8
13	3	3	-0.0	< 1.2