Acta Cryst. (1970). A**26**, 559

A Neutron Diffraction Study of Ferroelectric, KFCT, $K_4Fe(CN)_6 . 3D_2O$, above the Curie Temperature*

By J. C. Taylor,† M. H. Mueller and R. L. Hitterman

Argonne National Laboratory, Argonne, Illinois 60439, *U.S.A.*

(*Received* 14 *January* 1969)

A neutron diffraction study of deuterated potassium ferrocyanide trihydrate (KFCT) has been made above the ferroelectric Curie temperature. The monoclinic form, space group $A2/a$ (No. 15), has $a=9{\cdot}42$, $b=17{\cdot}01$, $c=9{\cdot}38$ Å, and $\beta=90{\cdot}03°$ at 20°C. Since all of the large crystals of KFCT were twinned by a 90° rotation about the b axis, data from both overlapped and nonoverlapped reflections were used in the determination of the structure. Refinement by a modified least-squares method that accounted for the overlapped data led to a weighted R value on F^2 (3678 reflections) of 4·8%. The corresponding R on F is 4·9%. The disordered water molecules are of two types: one is disordered into two positions related by a twofold axis parallel to **b**: the other is disordered into two positions that are related by an approximate 90° rotation in the plane of the molecule. Both types of water molecules show O–D $\cdots$ O or O–D $\cdots$ N bonding. The $Fe(CN)_6^{4-}$ octahedra are regular and the potassium ions are loosely surrounded by O and N atoms. This analysis has elucidated the role of the water molecules in the ferroelectric switching mechanism. The $[\bar{1}01]$ ferroelectric axis in this crystal can be explained on the basis of the dipole moment and orientation of the water molecule dipoles.

Introduction

An X-ray diffraction study of potassium ferrocyanide trihydrate (KFCT, hydrogen form) was made by Pospelov & Zhdanov (1947*a*). They reported that large single crystals were difficult to prepare because of twinning of the pseudotetragonal structure by a 90° rotation about **b**. Toyoda, Niizeki & Waku (1960) in a polarizing microscope study found at least three different types of twinning. However, all of the heavy atoms, except one water oxygen atom, were located by means of Patterson projections by Pospelov & Zhdanov (1947*b*). In an X-ray study Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) located the missing water oxygen atom.

Ferroelectric behavior in KFCT below $-24{\cdot}5$°C (or -18°C for the deuterated form) was discovered by Waku, Masuro & Tanaka (1959) and by Waku, Hirabayashi, Toyoda & Iwasaki (1959), and further studied by Waku, Masuro, Tanaka & Iwasaki (1960). The nuclear magnetic resonance (n.m.r.) studies of KFCT were carried out by Blinc, Brenman & Waugh (1961), by Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) and by Tsang & O'Reilly (1965). These studies agreed that the onset of ferroelectric behavior is connected with an ordering of the hydrogen-bonded water molecules. Blinc, Brenman & Waugh (1961) considered that the electronic and ionic polarizabilities of K^+ and $Fe(CN)_6^{4-}$ as well as displacements of K^+ ions contributed significantly to the internal field and spontaneous polarization. Structures for the ferroelectric phase were proposed in the three n.m.r. studies but these were all different.

Hazony, Earls & Lefkowitz (1968), based on Mössbauer studies, suggested that the mechanism is a mode instability (Cochran, 1960) and considered the K^+ ion to be vibrating against the $Fe(CN)_6^{4-}$ complex. They also stated that the water molecules have a substantial effect on the dynamics of the iron atom and provide the interaction between the balance of forces from K^+ to the $Fe(CN)_6^{4-}$ complex.

Since further clarification of the ferroelectric transition in KFCT depends, to a large extent, on the knowledge of the atomic positions, the present neutron diffraction study of the paraelectric phase was undertaken.

Experimental

The use of deuterated KFCT was preferred since (*a*) the deuterium atoms have a larger scattering length than hydrogen atoms for thermal neutrons, (*b*) the larger spin diffuse scattering by hydrogen results in considerable background, and (*c*) the measured linear absorption coefficient for the deuterated salt is $\mu=0{\cdot}44$ cm^{-1}, whereas it is 0·88 cm^{-1} for the hydrogen form.

The deuterated salt was prepared by dehydrating the normal salt at 110°C for 6 hours and dissolving the powder in 99·8% D_2O. Large crystals several mm on a side were grown by slow evaporation in a dry nitrogen atmosphere. The hydrogen content of the crystals was less than 0·5 mole per cent as checked by proton magnetic resonance.

---

* Based on work performed under the auspices of the U.S. Atomic Energy Commission.

† Present address: Australian Atomic Energy Research Establishment, Sutherland, N.S.W., Australia.

Most of the crystals had no marked extinction under polarized light; however, one crystal had good extinction throughout its volume, was optically biaxial, and appeared to be a monoclinic single crystal. The crystal was cooled to liquid nitrogen temperature to minimize extinction and to remove any tetragonal form (Toyoda, Niizeki & Waku, 1960). The crystal was shaped to a cylinder that had a diameter of 0·80 cm, a thickness of 0·37 cm, and the *b* axis along the cylinder axis.

Complete neutron diffraction data were collected at 20°C for 3678 reciprocal lattice points to $\sin\theta/\lambda = 0{\cdot}82$, with $\lambda = 1{\cdot}065$ Å. The data clearly indicated that the crystal was twinned (into two equal parts *A* and *B*) with *A* face centering and related by a 90° rotation about *b*. Since the monoclinic cell is practically tetragonal with $a \simeq c$ and $\beta \simeq 90°$, the overlap of reciprocal lattice points was almost exact. Some points in the composite reciprocal lattice were superposed reflections, others were single reflections, while others had no intensity, corresponding to face-centered absences. (See Fig. 1.) The reflection types are defined in Table 1.

Table 1. *Classification of reflection types in* KFCT

Number of *hkl*'s	Type*	Observed as
1148	*oee* *eoo*	Single reflections (*A*)
2530	*eee* *ooo*	Superposed $I_{\text{obs}} = I_{hkl}(A) + I_{\bar{l}kh}(B)$
3678		
~1200	*eeo* *ooe*	Single reflections (*B*)
——	*oeo* *eoe*	Absent due to *A* face-centering

* *e* – even
o – odd

The measured intensities for 27 nonsuperposed reflections from part *A* and the corresponding reflections from part *B* were summed. Since the sums differed by less than 0·3%, the crystal appeared to be a 50:50 twin. The peak profiles were well-defined as shown in Fig. 2(*a*) with equal integrated intensities from the reflections of parts *A* and *B*. For comparison, the scans of a typical twinned crystal with a twin ratio quite different from 1:1 are shown in Fig. 2(*b*).

The cell dimensions of KFCT were determined by using the least-squares lattice constant program of Mueller, Heaton & Miller (1960). Results from three sets of neutron data from approximately 17 reflections are shown in Table 2. The single reflections serve to differentiate the *a* and *c* dimensions, whereas this is not true for the overlapped reflections. The *a* and *c* axes of Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) have been interchanged to agree with the conventional $a > c$ for monoclinic crystals as proposed by Donnay (1963).

A very small fragment of the same KFCT crystal used for neutron diffraction was used to collect limited X-ray diffraction intensities. The volume ratio $A:B$ in this fragment was determined from X-ray intensities similar to that described above for neutrons. A value of approximately 3:1 was obtained as compared with 1:1 for the large crystal. This indicates that the twinning is not homogeneous.

Structure analysis

A three-dimensional Patterson synthesis of the neutron data gave the vector map of the superposed structures, and confirmed the positions for the Fe(CN)_6^{4-} proposed in the X-ray investigation by Pospelov & Zhdanov (1947*b*) and by Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964). The positions of the K^+ ion and the water molecules were not revealed in the synthesis. The K^+ locations as determined by these two groups of investigators were assumed to be reliable. The water atoms were located in the present study by

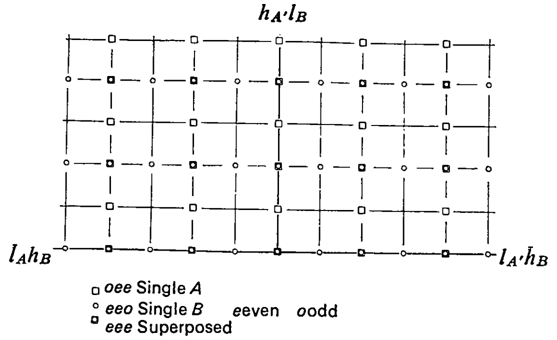


Fig. 1. Reciprocal lattice diagram for *k* even, illustrating the 90° twinning found in KFCT.

Table 2. *Lattice constants of KFCT, space group A*2/*a* (No. 15)

Reflections used	*a*	*b*	*c*	*β*
1	9·415 (7) Å	17·006 (13) Å	9·382 (7) Å	90·03 (2)°
2	9·420 (4)	17·040 (7)	9·396 (4)	90·08 (1)
3	9·428 (12)	16·937 (12)	9·437 (12)	90·07 (4)

1 Single reflections, part *A*.
2 Single reflections, part *B*.
3 Superposed reflections.

means of the following Fourier technique. The F^2 values were calculated for the K$^+$ and Fe(CN)$_6^{4-}$ contribution only; then the observed F^2 values for the overlapped reflections were divided up in the ratio of the twin components to derive approximations for $|F_{o(hkl)}|$ and $|F_{o(\bar{l}kh)}|$ as follows:

$$|F_{o(hkl)}| = \sqrt{\frac{F_o^2 \times F^2_{c(hkl)}}{F^2_{c(hkl)} + F^2_{c(\bar{l}hk)}}}$$

$$|F_{o(\bar{l}kh)}| = \sqrt{\frac{F_o^2 \times F^2_{c(\bar{l}kh)}}{F^2_{c(hkl)} + F^2_{c(\bar{l}kh)}}}$$

$$(F_o - F_c)_{hkl} = \frac{A_{hkl}}{|A_{hkl}|} \sqrt{\frac{F_o^2 \times F^2_{c(hkl)}}{F^2_{c(hkl)} + F^2_{c(\bar{l}kh)}}} - \frac{A_{hkl}}{|A_{hkl}|} \sqrt{F^2_{c(hkl)}}$$

$$(F_o - F_c)_{\bar{l}kh} = \frac{A_{\bar{l}kh}}{|A_{\bar{l}kh}|} \sqrt{\frac{F_o^2 \times F^2_{c(\bar{l}hk)}}{F^2_{c(hkl)} + F^2_{c(\bar{l}kh)}}} - \frac{A_{\bar{l}kh}}{|A_{\bar{l}kh}|} \sqrt{F^2_{c(\bar{l}kh)}} \,.$$

The above Fourier coefficients were used to calculate Fourier and difference Fourier syntheses that clearly revealed the disordered water molecules. The water molecule I, near the twofold axis associated with O(1), was found to be disordered (including the oxygen atoms) into half-atoms on each side of the twofold axis (Fig. 3). The water molecule II, in the general location associated with O(2) O(3), was also disordered into two overlapped pcsitions as shown in Fig. 4.

The initial model was refined on F^2 with the Kennicott (1963) modification of the least-squares program *ORFLS*, Busing, Martin & Levy (1962), which accounts for overlapped data. The number of F^2 values in the final cycles was 3678, and the value of

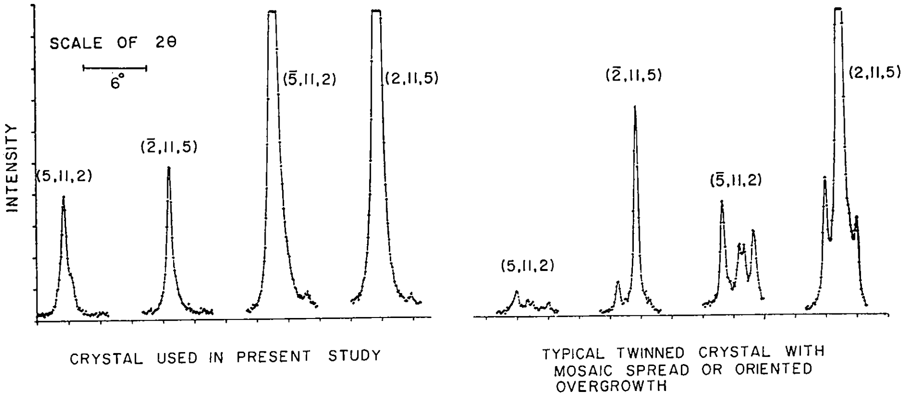
$$R = \frac{(\sum w(F_o - sF_c)^2)^{1/2}}{(\sum wF_o^2)^{1/2}}$$

was reduced to 4·6%; the value of w is given by the statistical weighting scheme of Evans (1961) where s is a scale factor.

The disordered positions for the oxygen atoms of water I were resolved in the Fourier syntheses and refined in the least-squares procedure; however, the half-oxygen atoms and superposed deuterium atoms of water II were too close to be resolved in the Fourier syntheses or refined by least-squares. Accordingly, the superposed oxygen and the superposed deuterium atoms of water II were refined as single atoms with double weight.

Fourier and difference Fourier syntheses were calculated from the final set of structure factors in the region of the water II molecule at $y=\frac{1}{2}$. The disordered atom sites in the overlapped peaks were estimated from the observed peak shapes. The theoretical shape for a half-oxygen or a half-deuterium atom was found by drawing the isotropic equivalent of a resolved half-deuterium [D(6) in this case]. The two theoretical half-atoms were then moved and their composite contours plotted until the composite curve fitted the observed peak shape. The observed and difference Fourier syntheses, on one-fifth the absolute scale, are shown at the $y=0{\cdot}500$ level in Fig. 5(*a*) and (*b*) together with the positions proposed for the superposed half-atoms, O(2), O(3), D(3), and D(5). Bond lengths for the disordered molecules in water II were normal to within the estimated errors (Table 4). The separations O(2)–O(3) and D(3)–D(5) were 0·35 ± 0·25 and 0·65 ± 0·35 Å. In view of the disorder separations, it was not surprising that these overlapped atoms failed to refine as individual atoms.

An R value on F was derived by splitting the F_o^2 values of the overlapped reflections as described above



(*a*) (*b*)

Fig. 2. Peak scans of 50:50 twin used in this study and scans of an unusable crystal exhibiting irregular peak shapes and a large mosaic spread.

The *R* value on *F* for the 3678 reflections was 4·9%. The good agreement between observed and calculated structure factors justified our decision to proceed with a structural analysis of the twinned crystal. The final positional and thermal parameters are given in Table 3.

Extinction effects were not severe in the intensity data; only 17 single reflections and 38 doubled reflections were omitted from the least-squares refinement and are designated by an asterisk in Table 5.

The interatomic distances and angles are listed in Table 4. A list of the final observed and calculated structure factors is given in Table 5.

Discussion

Potassium ions and $Fe(CN)_6^{4-}$ *groups*

Both potassium atoms K(1) and K(2) are loosely surrounded by oxygen and nitrogen atoms in an irregular fashion. K(1) has three oxygen atoms, one the disordered O(2)–O(3) atom, and four nitrogen atoms as nearest neighbors; K(2) is surrounded by one oxygen atom, the disordered O(2)–O(3) atom, and six nitrogen atoms. The K–O and K–N distances lie between 2·82 Å and 3·11 Å. (Table 4).

The octahedral $Fe(CN)_6^{4-}$ group is nearly regular (see Table 4).

Water molecules

The water I and water II molecules are highly disordered, as shown in Figs. 3 and 4. Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) reported that dynamic disordering may occur with a reorientation frequency greater than 10^5 cps. The half-oxygen atoms of water I, disordered about the twofold axis, are separated by 0·86 Å; the half-deuterium atoms nearest the twofold axis are separated by 0·54 Å. The distances and angles in water I are normal (Table 4).

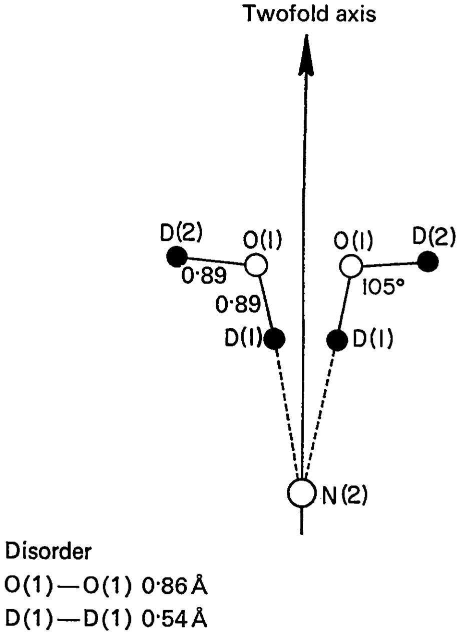


Fig. 3. Relative position of the disordered water molecule I found in KFCT.

Table 3. *Positional and thermal parameters*

The parameters and their standard deviations are multiplied by 10^4. The temperature factor expression is

$$\text{T.F.} = \exp\left[-(\beta_{11}h^2 + 2\beta_{12}hk + 2\beta_{13}hl + \beta_{22}k^2 + 2\beta_{23}kl + \beta_{33}l^2)\right].$$

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Fe	2500	1765 (2)	0	0027 (2)	0016 (1)	0029 (2)	0	0001 (2)	0
N(1)	2500	−0053 (1)	0	0084 (4)	0012 (1)	0182 (6)	0	0047 (4)	0
N(2)	2500	3598 (2)	0	0067 (5)	0019 (5)	0099 (5)	0	0014 (4)	0
N(3)	1390 (2)	1748 (2)	6924 (2)	0060 (2)	0040 (1)	0038 (2)	0002 (2)	−0013 (1)	−0014 (1)
N(4)	4394 (2)	3219 (2)	6101 (2)	0044 (2)	0033 (1)	0071 (2)	−0013 (1)	0011 (1)	0006 (1)
C(1)	2500	0643 (2)	0	0062 (5)	0023 (1)	0066 (5)	0	0006 (5)	0
C(2)	2500	2915 (2)	0	0054 (4)	0012 (1)	0024 (4)	0	−0006 (4)	0
C(3)	1806 (2)	1774 (2)	8076 (2)	0039 (2)	0021 (1)	0034 (2)	0003 (1)	−0002 (1)	−0005 (1)
C(4)	4419 (2)	1778 (2)	9325 (2)	0033 (2)	0021 (1)	0040 (2)	−0008 (1)	0003 (1)	0002 (1)
K(1)	4350 (5)	1431 (3)	5963 (6)	0050 (5)	0034 (3)	0050 (5)	−0019 (2)	−0018 (3)	0001 (2)
K(2)	1576 (6)	3574 (3)	6907 (5)	0043 (5)	0049 (3)	0056 (6)	0007 (3)	−0015 (4)	−0021 (3)
O(1)	2276 (10)	0242 (4)	5391 (8)	0133 (10)	0016 (2)	0093 (8)	−0007 (4)	0023 (6)	0000 (3)
D(1)	2275 (11)	−0272 (4)	5176 (13)	0096 (12)	0030 (2)	0150 (12)	0016 (4)	0041 (8)	0037 (6)
D(2)	1702 (13)	0283 (6)	6144 (14)	0393 (26)	0037 (3)	0209 (16)	0012 (8)	0046 (16)	−0010 (6)
O(2)	0030 (130)	0000 (70)	7750 (130)	disordered atom – coordinates from Fourier synthesis					
D(3)	0780 (190)	0060 (110)	8300 (190)	disordered atom – coordinates from Fourier synthesis					
D(4)	−0784 (16)	−0214 (6)	8376 (12)	0554 (41)	0059 (4)	0168 (13)	−0096 (12)	−0055 (22)	0015 (7)
O(3)	0190 (130)	−0050 (70)	7500 (130)	disordered atom – coordinates from Fourier synthesis					
D(5)	0690 (190)	−0230 (110)	8300 (190)	disordered atom – coordinates from Fourier synthesis					
D(6)	0926 (17)	0281 (10)	7042 (25)	0391 (32)	0095 (8)	0524 (49)	−0104 (13)	−0010 (33)	0121 (16)
O(2)*	0164 (6)	−0013 (5)	7604 (7)	0191 (9)	0037 (2)	0257 (10)	−0024 (3)	−0100 (10)	0028 (3)
D(3)*	0675 (8)	−0087 (5)	8316 (5)	0337 (14)	0122 (5)	0122 (6)	0100 (7)	−0029 (9)	−0003 (4)

O(2)* is a composite of the superposed O(2) and O(3) in Water II.
D(3)* is a composite of the superposed D(3) and D(5) in Water II.

Water II, disordered by a 90° rotation in the plane of the molecule, is shown in Fig. 4. The half-oxygen atoms are disordered by 0·35 ± 0·25 Å and the half-deuterium atoms by 0·65 ± 0·35 Å. The dimensions of the overlapped molecules are normal, within the estimated errors (Table 4).

The arrangement of water molecules found by our neutron study is in agreement with the nuclear magnetic resonance (n.m.r.) study by Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) carried out at −170° C. The relation between the present results and the n.m.r. results is discussed in the section on ferroelectricity. The present results are in disagreement with the earlier n.m.r. study of Tsang & O'Reilly (1965) but agree with their later interpretation (O'Reilly & Tsang, 1967).

Deuterium bonding

(*a*) *Water* I

One deuterium, D(1), forms a bond with a length 2·84 Å with N(2) on the twofold axis, Fig. 3 and Table 4. The other deuterium, D(2), forms a bond with a length 2·83 Å with O(3) and has a much weaker possible interaction with N(3) with a distance of 3·05 Å. (See lower portion of Fig. 4).

(*b*) *Water* II

Deuterium bonding around water II is shown in Fig. 4. For the half-molecule D(3)–O(2)–D(4) the following possible O–D···N distances are observed: 3·14, 3·19, and 3·26 Å. These distances suggest weak hydrogen bonding. In the half-molecule D(5)–O(3)–D(6), possible deuterium bonding distances of 2·83, 3·20, 3·25, and 3·31 Å occur.

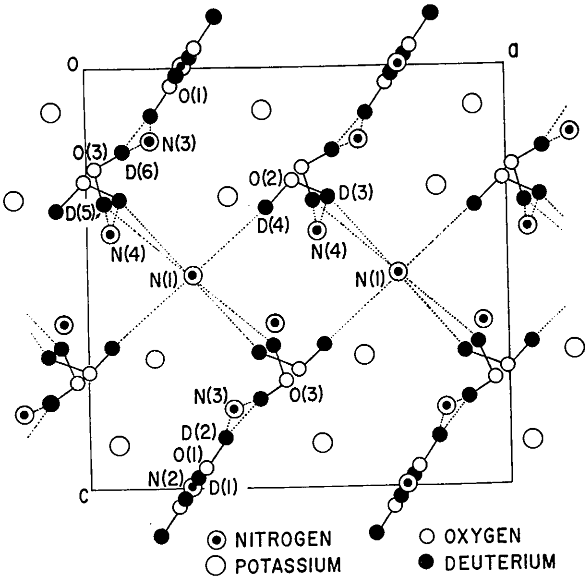


Fig. 4. The *a–c* projection of KFCT near $y = 0·5$ showing the disordered water molecules and possible hydrogen bonding.

A complete distance and angle tabulation for possible deuterium bonding is given in Table 4. The deuterium bonding in the crystal is generally weak and the deuterium bonds are continually being made and broken in the disorder flipping, which is directly related to the ferroelectric switching.

Ferroelectricity in KFCT

If we combine the present neutron diffraction study of the paraelectric phase, which is disordered, with the n.m.r. study by Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) (carried out at −170° C, where the water molecules are rigid) the role of the water molecules in the ferroelectric transition becomes evident. The room temperature arrangement of disordered water molecules, Fig. 4, is equivalent to the

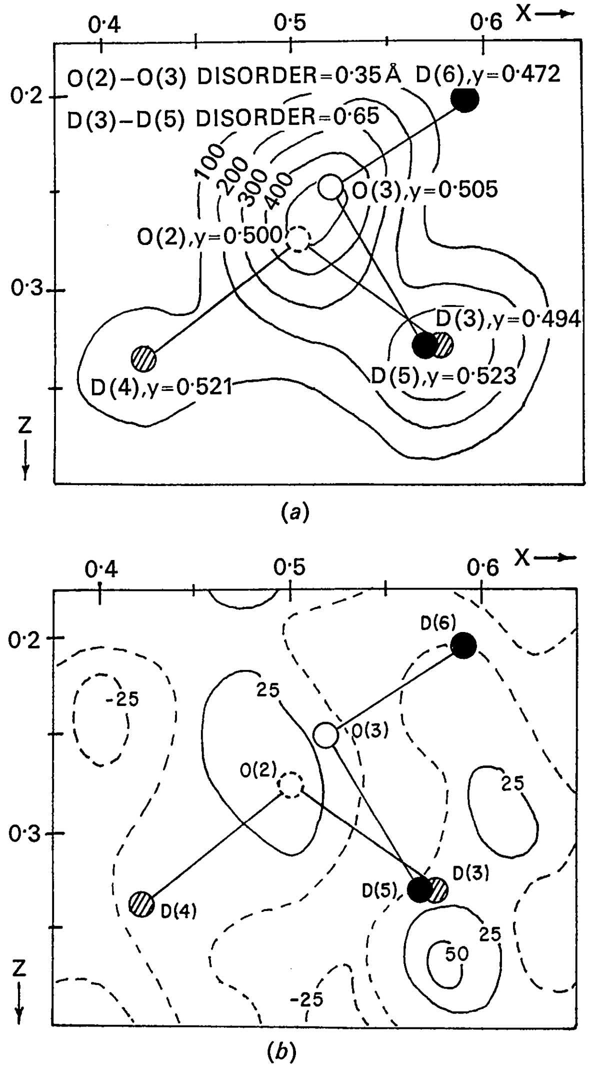


Fig. 5. (*a*) Observed Fourier section at $y = 0·5$ showing disordered water molecule II. (*b*) A difference Fourier section at $y = 0·5$ in the vicinity of water molecule II.

superposed ferroelectric structures proposed by Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964). In one low-temperature ferroelectric state, the water molecule II splits into two non-equivalent water molecules associated with O(2) and O(3) and the space group becomes *Aa* (No. 9). One ferroelectric state is denoted by the solid arrow water dipoles corresponding to O(2) and O(3) in Fig. 6. The other ferroelectric state is denoted by the dashed arrows. The water molecule I is no longer associated with a twofold axis and assumes that one of the room temperature orientations which is dictated by steric requirements.

The definition of the ferroelectric axis arises naturally from the foregoing results since the dipole moment of a water molecule bisects the D–O–D angle in the plane of the molecule. The ferroelectric axis in this crystal is the [$\bar{1}$01] since the moments associated with the water molecules of O(2) and O(3) are directed with one along [001] and the other along [$\bar{1}$00], as shown by the dashed arrows in Fig. 6. In a similar manner the solid arrows correspond to a [10$\bar{1}$] direction. The water I moment is forced to align in the same direction as the O(2), O(3) resultant. In the averrage structure above the Curie temperature, the water moments cancel.

Kiriyama, Kiriyama, Wada, Niizeki & Hirabayashi (1964) and Blinc, Brenman & Waugh (1961) agree that deviations from the ordered structure begin at − 140°C.

Table 4. *Interatomic distances and bond angles*

Ferrocyanide groups

Standard deviations ($\times 10^3$) for distances and ($\times 10^2$) for angles are in parentheses.

Fe —C(1)	1·908 (4) Å	N(1)–C(1)–Fe	180·0°
Fe —C(2)	1·956 (4)	N(2)–C(2)–Fe	180·0
Fe —C(3)	1·920 (2)	N(3)–C(3)–Fe	177·38 (38)
Fe —C(4)	1·915 (2)	N(4)–C(4)–Fe	179·48 (55)
C(1)–N(1)	1·184 (3)	C(1)–Fe —C(3)	90·12 (3)
C(2)–N(2)	1·147 (3)	C(1)–Fe —C(4)	90·14 (3)
C(3)–N(3)	1·150 (2)	C(3)–Fe —C(4)	90·55 (10)
C(4)–N(4)	1·187 (2)	C(2)–Fe —C(3)	89·88 (3)
		C(2)–Fe —C(4)	89·86 (3)

Potassium contacts

Standard deviations ($\times 10^3$) are in parentheses.

K(1)–O(2)	*3·020 (100) Å	K(2)–O(2)	*2·880 (100) Å
K(1)–O(3)	*2·870 (100)	K(2)–O(3)	*3·060 (100)
K(1)–N(3)	2·979 (5)	K(2)–N(4)	2·824 (6)
K(1)–O(1)	2·862 (9)	K(2)–N(2)	3·029 (5)
K(1)–O(1)	2·836 (10)	K(2)–N(3)	3·050 (6)
K(1)–N(3)	2·848 (6)	K(2)–N(4)	3·026 (5)
K(1)–N(2)	3·101 (5)	K(2)–N(1)	3·067 (6)
K(1)–N(4)	3·043 (6)	K(2)–N(3)	3·109 (7)

* Superimposed half oxygen atoms.

Water molecules

Standard deviations ($\times 10^2$) for distance and ($\times 1$) for angles are in parentheses

O(1)–D(1)	0·90 (1) Å	O(3)–D(5)	0·94 (10) Å
O(1)–D(2)	0·89 (1)	O(3)–D(6)	0·99 (10)
D(1)–O(1)–D(2)	105·00 (1)°	D(5)–O(3)–D(6)	101·00 (14)°
O(2)–D(3)	0·88 (10) Å		
O(2)–D(4)	1·03 (10)		
D(3)–O(2)–D(4)	108·00 (14)°		

Hydrogen bonds

Standard deviations ($\times 10^2$) for distances and ($\times 1$) for angles are in parentheses

O(1)–N(2)	2·84 (1) Å	O(2)–N(4)	3·26 (10) Å
D(1)–N(2)	1·96 (1)	D(3)–N(4)	3·19 (17)
O(1)–D(1)–N(2)	170·00 (1)°	O(2)–D(3)–N(4)	87·00 (12)°
O(1)–O(3)	2·83 (10) Å	O(3)–O(1)	2·83 (10) Å
D(2)–O(3)	1·99 (17)	D(6)–O(1)	2·00 (2)
O(1)–D(2)–O(3)	156·00 (14)°	O(3)–D(6)–O(1)	140·00 (6)°
O(1)–N(3)	3·05 (1) Å	O(3)–N(1)	3·20 (10) Å
D(2)–N(3)	2·61 (1)	D(5)–N(1)	2·35 (17)
O(1)–D(2)–N(3)	111·00 (1)°	O(3)–D(5)–N(1)	150·00 (14)°
O(2)–N(1)	3·14 (10) Å	O(3)–N(4)	3·25 (10) Å
D(3)–N(1)	2·28 (17)	D(5)–N(4)	2·70 (17)
O(2)–D(3)–N(1)	166·00 (15)°	O(3)–D(5)–N(4)	118·00 (14)°
O(2)–N(1)	3·19 (10) Å	O(3)–N(3)	3·31 (10) Å
D(4)–N(1)	2·29 (2)	D(6)–N(3)	2·54 (2)
O(2)–D(4)–N(1)	147·00 (14)°	O(3)–D(6)–N(3)	134·00 (6)°

Above −40°C a sudden increase in the reorientation frequency of the water molecules occurs. They also agree that no very large shifts in the heavier atoms occur at the Curie point of −18°C. Blinc, Brenman & Waugh (1961) consider that electronic and ionic polarizabilities of K^+ and $Fe(CN)_6^{4-}$ and some displacement of the K^+ ions could contribute significantly to the internal field and spontaneous polarization. The

Table 5. *Observed and calculated structure factors* (× 10)

The first part of the Table contains the single reflections and the second part contains the overlapped reflections. The column headed $F^2C(S) = F^2C(HKL) + F^2C(\bar{L}KH)$. Reflections indicated with an asterisk presumably suffer from extinction and were omitted from the final least-squares refinement.

L	F²O	F²C
H= 0, K= 1		
-11	47	74
-9	0	14
-7	84	72
-5	172	190
-3	273	385
1	345	321
3	220	385
5	154	190
7	77	72
9	15	14
11	53	74
13	42	41
H= 0, K= 3		
-11	0	61
-9	2	3
-7	462	407
-5	1600	1682
-3	1	16
-1	247	305
3	53	16
5	1576	1682
7	474	407
9	0	3
11	19	61
13	6	12
H= 0, K= 5		
-11	21	8
-9	11	24
-7	65	12
-5	252	174
-3	33	107
-1	920	1095
1	973	1095
3	33	107
5	225	174
7	29	12
9	25	24
11	16	8
13	17	22
H= 0, K= 7		
-11	14	13
-9	116	95
-7	0	37
-5	279	264
-3	406	308
1	0	14
3	371	308
5	278	264
7	0	37
9	122	95
11	48	13
13	27	6
H= 0, K= 9		
-11	136	116
-9	241	210
-7	138	41
-5	131	146
-3	342	335
-1	771	845
1	745	845
3	335	335
5	193	146
7	59	41
9	245	210
11	162	116
H= 0, K= 11		
-11	181	161
-9	655	639
-7	93	93
-5	8	0
-3	727	681
* -1	1936	4410
* 1	3927	4410
3	760	681
5	5	0
7	124	93
9	688	639
11	177	181
H= 0, K= 13		
-9	78	3
-7	36	135
-5	452	345
-3	0	6
-1	9	24
1	81	24
3	18	6
5	351	345
7	31	135
9	106	3
11	0	0
H= 0, K= 15		
-9	9	14
-7	0	14
-5	199	166
-3	0	1
-1	0	1
1	0	1
3	41	1
5	172	166
7	13	14
9	25	14
H= 0, K= 17		
-7	175	241
-5	124	226
-3	1093	1056
* -1	2975	3978
* 1	3129	3978
3	1095	1056
5	131	226
7	203	241
9	647	500
H= 0, K= 19		
-5	45	19
-3	0	39
-1	0	4
1	0	4
3	0	39
5	50	19
7	46	17
H= 0, K= 21		
-5	86	53
-3	0	11
-1	0	28
1	0	28
3	0	11
5	80	53
H= 0, K= 23		
-3	102	28
-1	232	396
* 1	123	396
3	94	28
H= 1, K= 2		
-12	23	8
-10	270	252
-8	266	339
-6	29	54
-4	128	27
-2	1697	1768
0	668	658
2	137	133
4	178	145
6	69	37
8	805	738
10	143	152
12	20	12
H= 1, K= 4		
-12	0	12
-10	298	290
-8	266	339
-6	202	164
-4	270	165
-2	2345	2394
0	178	231
2	0	1
4	804	724
6	105	117
8	2338	2347
10	116	104
H= 1, K= 6		
-12	58	59
-10	212	165
-8	63	73
-6	242	208
-4	109	11
-2	1631	1665
* 0	775	995
2	835	787
4	146	76
6	272	111
8	409	434
10	30	9
12	52	12
H= 1, K= 8		
-10	122	146
-6	35	18
-4	107	0
-2	730	798
0	480	566
2	154	166
4	0	3
6	14	20
8	82	80
10	69	115
12	29	0
H= 1, K= 10		
-10	1495	1416
-8	90	78
-6	1948	1845
-4	441	570
-2	123	142
* 0	2223	2441
2	1237	1336
4	3692	3681
6	1876	1843
8	558	518
10	761	808
12	273	263
H= 1, K= 12		
-10	295	304
-8	44	79
-6	393	444
-4	0	3
-2	1574	1667
* 0	593	873
2	477	627
4	249	313
6	227	142
8	696	604
10	0	5
H= 1, K= 14		
-8	94	10
-6	0	9
-4	38	1
-2	58	87
0	0	58
2	0	8
4	53	22
6	0	7
8	40	9
10	11	17
H= 1, K= 16		
-8	38	87
-6	859	728
-4	294	389
-2	50	38
0	1341	1472
* 2	670	904
4	1520	1567
6	824	875
8	115	144
10	330	394
H= 1, K= 18		
-6	451	654
-4	0	61
-2	134	76
* 0	617	795
2	441	521
4	583	901
6	285	368
8	85	29
H= 1, K= 20		
-4	0	8
-2	47	4
0	35	18
2	57	12
4	0	19
6	6	0
H= 1, K= 22		
-2	17	25
0	112	206
2	10	96
4	182	115
H= 1, K= 24		
-2	133	142
0	2	8
2	34	2
H= 2, K= 1		
-11	519	488
-9	16	31
-7	101	140
-5	8	1
-3	33	35
-1	306	244
1	2060	2164
3	721	645
5	486	431
7	13	7
9	165	271
11	0	1
13	33	0
H= 2, K= 3		
-11	883	951
-9	716	635
-7	93	31
-5	16	8
-3	1866	1788
-1	7	2
1	858	817
3	178	140
5	1637	1657
7	205	193
9	78	51
11	564	561
13	81	53
H= 2, K= 5		
-11	627	534
-9	167	184
-7	336	347
-5	37	6
-3	61	22
-1	463	424
1	4479	4578
3	936	597
5	1578	1576
7	9	19
9	424	472
11	391	364
13	54	129
H= 2, K= 7		
-11	29	56
-9	63	71
-7	0	0
-5	53	82
-3	47	33
1	28	39
3	146	57
5	71	49
7	0	18
9	94	0
11	34	80
H= 2, K= 9		
-11	1155	1251
-9	36	9
-7	666	485
-5	462	409
-3	36	16
-1	399	430
1	421	500
3	253	197
5	2371	2237
7	51	30
9	802	670
11	66	52
H= 2, K= 11		
-9	42	29
-7	1505	1475
-5	722	722
-3	667	537
* -1	1737	2123
1	420	515
3	1826	1840
5	4181	4082
7	372	365
9	1133	1199
11	124	98
H= 2, K= 13		
-9	72	65
-7	21	17
-5	0	1
-3	58	68
-1	0	141
1	838	901
3	82	182
5	0	72
7	15	24
9	117	11
11	38	112
H= 2, K= 15		
-9	0	12
-7	98	101
-5	24	40
-3	0	10
-1	71	12
1	966	859
3	0	1
5	258	307
7	5	0
9	185	197
H= 2, K= 17		
-7	1267	1149
-5	851	987
-3	663	614
* -1	1860	2178
1	0	84
3	1587	1846
5	3096	3038
7	527	642
9	821	910
H= 2, K= 19		
-5	0	23
-3	149	55
-1	0	35
1	306	414
3	58	28
5	104	208
7	9	0
H= 2, K= 21		
-3	0	4
-1	0	6
1	80	189
3	0	36
5	22	0
H= 2, K= 23		
-3	0	1
-1	311	169
1	88	4
3	77	131
H= 3, K= 2		
-12	23	11
-10	8	1
-8	403	424
-6	77	60
-4	120	122
-2	90	92
0	140	123
2	275	276
4	76	63
6	0	18
8	546	501
10	100	60
12	41	13
H= 3, K= 4		
-12	70	54
-10	67	76
-8	320	244
-6	20	10
-4	37	17
-2	75	18
0	38	36
2	918	634
4	963	957
6	24	2
8	915	1007
10	39	16
12	72	19
H= 3, K= 6		
-12	17	12
-10	97	124
-8	117	68
-6	63	39
-4	22	2
-2	177	203
0	143	88
2	167	51
4	200	137
6	41	0
8	315	268
10	61	39
12	39.	1
H= 3, K= 8		
-12	0	3
-10	57	8
-8	204	284
-6	62	50
-4	53	48
-2	35	30
0	71	79
2	15	13
4	14	5
6	5	23
8	131	113
10	71	73
12	50	6
H= 3, K= 10		
-12	112	95
-10	811	928
-8	1419	1311
-6	469	508
-4	972	780
-2	1558	1700
0	1090	1160
2	203	217
4	31	8
6	987	878
8	2732	2720
10	673	632
12	139	235
H= 3, K= 12		
-10	181	213
-8	103	160
-6	10	18
-4	0	19
-2	53	125
0	139	92
2	0	0
4	169	166
6	4	0
8	630	515
H= 3, K= 14		
-8	102	50
-6	17	7
-4	0	11
-2	122	5
0	11	6
2	121	8
4	0	8
6	16	3
8	29	0
10	3	8
H= 3, K= 16		
-8	666	664
-6	292	344
-4	381	230
-2	960	1059
0	446	657
2	235	248
4	0	22
6	476	433
8	1160	982
H= 3, K= 18		
-6	7	221
-4	202	222
-2	252	327
0	200	255
2	0	13
4	84	32
6	34	153
8	735	699
H= 3, K= 20		
-4	0	24
-2	0	6
0	195	0
2	0	15
4	0	23
6	0	0
H= 3, K= 22		
-2	6	102
0	0	11
2	0	23
4	0	2
H= 4, K= 1		
-11	36	35
-9	21	0
-7	127	103
-5	428	461
-3	119	72
-1	59	17
1	225	172
3	249	160
5	27	6
7	154	45
9	464	482
11	63	70
H= 4, K= 3		
-11	83	111
-9	1166	1221
-7	224	282
-5	257	209
-3	1008	990
-1	439	472
1	881	653
3	56	16
5	214	154
7	1423	1521
9	335	347
11	336	283
H= 4, K= 5		
-11	2	7
-7	648	645
-5	689	681
-3	241	236
-1	333	241
1	128	94
3	29	14
5	91	32
7	1209	1097
9	544	455
11	250	208
H= 4, K= 7		
-11	0	0
-9	4	4
-7	109	158
-5	60	8
-3	212	145
-1	142	109
1	0	4
3	162	147
5	132	14
7	15	38
9	58	124
11	32	6
H= 4, K= 9		
-11	125	60
-9	13	88
-7	1031	987
-5	897	802
-3	92	27
-1	1242	1230
1	7	1
3	89	103
5	153	121
7	116	282
9	700	705
11	687	650
H= 4, K= 11		
-11	79	112
-9	113	1963
-5	1860	1899
-3	0	0
-1	1768	1826
1	845	885
3	1024	995
7	415	403
9	1237	1143
11	687	667
H= 4, K= 13		
-9	0	42
-7	129	138
-5	0	0
-5	372	306
-1	29	1
1	91	224
3	70	53
5	5	102
7	202	198
9	0	11
H= 4, K= 15		
-9	45	7
-7	244	215
-5	35	154
-3	145	69
-1	112	150
1	27	74
3	0	2
5	0	3
7	277	239
9	135	113
H= 4, K= 17		
-7	1290	1335
-5	1434	1501
-3	232	304
-1	1669	1798
1	1070	1124
3	1199	1376
5	1034	968
7	0	1
H= 4, K= 19		
-5	14	68
-3	16	22
-1	101	30
1	220	138
3	0	21
5	38	50
7	13	31
H= 4, K= 21		
-5	0	13
-3	68	18
-1	0	0
1	8	60
3	39	10
5	0	5
H= 4, K= 23		
-1	99	162
1	3	40
H= 5, K= 2		
-12	720	573
-10	546	473
-8	109	94
-6	0	5
-4	76	65
-2	1346	1330
0	223	225
2	18	21
4	533	477
6	880	882
8	7	19
10	103	72
12	40	39
H= 5, K= 4		
-10	1090	1137
-8	113	122
-6	37	45
-4	51	31
-2	1856	1887
0	853	868
2	18	3
4	273	380
6	972	1214
8	38	20
10	364	401
12	0	1
H= 5, K= 6		
-12	92	29
-10	308	305
-8	14	1
-6	32	16
-4	173	216
-2	718	618
0	431	389
2	140	119
4	507	358
6	58	46
8	190	113
10	151	204
12	23	24
H= 5, K= 8		
-10	81	48
-8	31	13
-6	0	1
-4	3	64
-2	470	517
0	11	71
2	45	62
4	224	237
6	193	235
8	37	42
10	0	1
H= 5, K= 10		
-10	179	169
-8	229	223
-6	374	508
-4	1005	1036
-2	4566	4446
0	31	9
2	985	884
4	2036	1948
6	15	0
8	972	925
10	0	22
H= 5, K= 12		
-8	70	7
-6	17	28
-4	75	102
-2	1268	1251
0	544	495
2	167	61
4	471	404
6	80	98
8	105	124
10	155	152
H= 5, K= 14		
-8	11	2
-6	0	4
-4	15	42
-2	0	93
0	47	64
2	5	10
4	0	9
6	11	13
8	0	9
H= 5, K= 16		
-8	136	115
-6	276	152
-4	443	586
-2	1945	1880
0	7	69
2	592	547
4	1042	942
6	0	37
8	628	538
H= 5, K= 18		
-4	117	189
-2	1530	1541
0	91	0
2	248	189
4	500	477
6	43	1
H= 5, K= 20		
-2	0	0
0	0	21
2	14	2
4	33	16
H= 5, K= 22		
-2	88	213
0	0	9
2	0	49
H= 6, K= 1		
-11	129	72
-9	161	244
-7	99	53
-5	97	68
-3	27	32
-1	279	287
1	233	63
3	70	150
5	20	0
7	281	319
9	45	45
11	7	0
H= 6, K= 3		
-11	50	15
-9	209	86
-7	845	677
-5	1797	1898
-3	79	9
-1	83	102
1	28	134
3	0	1
5	52	57
7	34	37
9	86	152
11	343	374
H= 6, K= 5		
-11	232	276
-9	190	123
-7	135	126
-5	266	273
-3	35	28
-1	621	757
1	518	293
3	50	6
5	0	16
7	403	461
9	127	120
11	53	5
H= 6, K= 7		
-11	38	43
-9	44	34
-7	78	98
-5	61	20
-3	0	41
-1	50	46
1	114	42
3	70	120
5	29	0
7	16	30
9	103	27
11	0	1
H= 6, K= 9		
-9	552	541
-7	63	2
-5	163	180
-3	429	350
-1	213	224
1	690	765
3	30	78
5	97	100
7	355	311
9	43	32
11	8	1
H= 6, K= 11		
-9	366	390
-7	15	16
-5	10	5
-3	392	515
-1	2171	2156
1	1778	1585
3	287	316
5	223	202
7	1163	1119
9	26	35
H= 6, K= 13		
-7	84	98
-5	97	137
-3	13	2
-1	0	6
1	0	0
3	190	158
5	25	97
7	0	22
9	37	1
H= 6, K= 15		
-7	0	2
-5	123	61
-3	0	34
-1	0	15
1	91	141
3	0	51
5	42	0
7	0	15
H= 6, K= 17		
-5	44	10
-3	848	620
-1	1828	1716
1	1383	1512
3	985	1034
5	399	428
7	950	833
H= 6, K= 19		
-3	7	16
-1	0	20
1	0	5
3	0	21
5	0	16
H= 6, K= 21		
-3	46	0
-1	0	10
1	0	4
3	106	76
H= 7, K= 2		
-10	3	1
-8	349	314
-6	140	165
-4	554	557
-2	183	123
0	40	25
2	71	59
4	13	298
6	34	22
8	223	262
10	30	25
H= 7, K= 4		
-10	21	12
-8	780	679
-6	132	107
-4	1844	1828
-2	106	102
0	247	206
2	203	140
4	419	449
6	473	474
8	143	165
10	0	17
H= 7, K= 6		
-10	0	0
-8	338	428
-6	88	52
-4	311	348
-2	0	1
0	0	34
2	188	342
4	103	333
6	107	124
8	9	15
10	34	4
H= 7, K= 8		
-8	129	73
-6	21	93
-4	18	23
-2	107	78
0	0	0
2	46	9
4	50	131
6	18	4
8	222	210
10	17	39
H= 7, K= 10		
-10	59	135
-8	2282	2166
-6	1083	1021
-4	291	244
-2	496	481
0	193	118
2	1953	1833
4	2289	2264
6	19	9
8	808	822
10	355	353
H= 7, K= 12		
-6	111	91
-4	571	547
-2	2	16
0	9	6
2	343	413
4	564	422
6	179	114
8	109	63
H= 7, K= 14		
-8	0	0
-6	0	22
-4	46	9
-2	0	27
0	4	1
2	0	9
4	52	7
6	0	11
8	21	18
H= 7, K= 16		
-6	481	546
-4	0	11
-2	333	245
0	144	64
2	1021	1094
4	1100	1230
6	35	8
H= 7, K= 18		
-4	45	38
-2	31	26
0	48	42
2	553	478
4	494	499
H= 7, K= 20		
-2	0	3
0	0	0
2	0	36
H= 8, K= 1		
-9	114	121
-7	260	301
-5	56	43
-3	574	655
-1	127	111
1	32	0
3	388	206
5	1	4
7	63	129
9	83	100
H= 8, K= 3		
-9	0	1
-7	145	75
-5	47	32
-3	455	410
-1	2009	2153
1	795	1006
3	228	316
5	356	595
7	944	768
9	57	76
H= 8, K= 5		
-9	124	124
-7	186	316
-5	176	207
-3	1107	1016
-1	1444	1402
1	208	52
3	351	332
5	18	6
7	542	581
9	17	12
H= 8, K= 7		
-7	11	1
-5	64	110
-3	0	19
-1	48	22
1	0	0
3	0	3
5	10	3
7	128	33
9	78	135
H= 8, K= 9		
-9	235	229
-7	597	380
-5	301	303
-3	1005	1114
-1	291	362
1	0	34
3	777	635
5	0	1
7	1445	1319
9	33	0
H= 8, K= 11		
-9	374	318
-7	484	624
-5	778	726
-3	2225	2079
-1	660	618
1	31	43
3	941	979
5	352	387
7	1590	1678
9	56	13
H= 8, K= 13		
-7	46	38
-5	35	54
-3	38	0
-1	243	305
1	142	158
3	75	5
5	45	36
7	165	52
H= 8, K= 15		
-7	174	79
-5	137	152
-3	179	366
-1	322	155
1	106	52
3	122	36
5	96	20
7	330	326
H= 8, K= 17		
-5	597	541
-3	1489	1622
-1	41	17
1	146	169
3	957	830
5	463	518
H= 8, K= 19		
-1	103	130
H= 9, K= 2		
-10	60	57
-8	0	1
-6	91	71
-4	672	579
-2	108	67
0	0	12
2	68	55
4	489	430
6	271	278
8	70	5
10	18	8
H= 9, K= 4		
-8	69	39
-6	123	131
-4	628	574
-2	120	107
0	13	10
2	479	507
4	964	913
6	118	225
8	16	4
H= 9, K= 6		
-8	0	6
-6	33	8
-4	119	155
-2	341	486
0	67	43
2	151	161
4	73	34
6	87	73
8	19	40
H= 9, K= 8		
-8	54	24
-6	42	19
-4	190	175
-2	53	34
0	0	18
2	0	0
4	69	57
6	175	124
8	49	7
H= 9, K= 10		
-8	0	75
-6	88	89
-4	1707	1559
-2	1381	1318
0	852	879
2	0	3
4	67	31
6	743	782
8	467	431
H= 9, K= 12		
-6	82	0
-4	175	269
-2	513	515
0	130	29
2	251	183
4	134	158
6	174	93
H= 9, K= 14		
-6	3	6
-4	61	1
-2	0	0
0	0	15
2	0	2
4	0	6
6	0	0
H= 9, K= 16		
-4	739	656
-2	847	761
0	380	641
2	50	22
4	0	0
H= 9, K= 18		
0	284	104
H= 10, K= 1		
-9	0	22
-7	46	90
-5	27	22
-3	104	105
-1	149	259
1	153	129
3	80	144
5	83	52
7	15	58
9	36	35
H= 10, K= 3		
-9	31	11
-7	0	3
-5	451	445
-3	6	1
-1	94	25
1	229	117
3	0	5
5	836	794
7	80	99
9	54	45
H= 10, K= 5		
-7	53	46
-5	212	97
-3	123	174
-1	114	215
1	444	492
3	233	256
5	859	806
7	11	6
H= 10, K= 7		
-7	9	0
-5	29	42
-3	23	21
-1	0	5
1	66	47
3	0	3
5	0	24
7	9	45
H= 10, K= 9		
-7	111	130
-5	0	1
-3	385	257
-1	390	238
1	786	695
3	280	209
5	50	155
7	38	7
H= 10, K= 11		
-5	78	16
-3	459	484
-1	467	491
1	1304	1378
3	843	839
5	401	352
H= 10, K= 13		
-5	18	59
-3	39	30
-1	0	0
1	41	43
3	0	22
H= 10, K= 15		
-3	103	41
-1	24	16
1	157	224
3	19	72
H= 11, K= 2		
-6	146	188
-4	286	308
-2	185	157
0	0	2
2	985	960
4	8	36
6	82	116
H= 11, K= 4		
-6	242	208
-4	351	279
-2	646	572
0	3	2
2	865	934
4	26	46
6	182	171
H= 11, K= 6		
-6	26	40
-4	104	165
-2	178	101
0	60	47
2	244	213
4	12	34
6	182	121
H= 11, K= 8		
-6	0	51
-4	85	131
-2	4	18
0	38	6
2	398	323
4	0	1
6	22	97
H= 11, K= 10		
-4	1139	993
-2	36	33
0	343	297
2	1678	1584
4	231	227
H= 11, K= 12		
-4	206	254
-2	240	153
0	48	29
4	54	27
H= 11, K= 14		
0	40	2
H= 12, K= 1		
-5	101	89
-3	10	1
-1	12	39
1	93	110
3	0	0
5	384	504
H= 12, K= 3		
-5	0	0
-3	105	251
-1	17	21
1	0	21
3	98	128
5	602	605
H= 12, K= 5		
-5	19	23
-3	12	26
-1	15	36
1	12	1
3	71	6
5	505	646
H= 12, K= 7		
-3	41	76
-1	40	5
1	79	48
3	36	5
5	58	65
H= 12, K= 9		
-3	34	10
-1	103	105
1	73	24
3	47	5
H= 12, K= 11		
-1	245	207
1	59	60
H= 13, K= 2		
-2	17	9
0	26	3
2	5	5
H= 13, K= 4		
-2	81	102
0	17	0
2	31	4
H= 13, K= 6		
0	80	101
2	48	58

L	F²O	F²C	F²C(S)
H= 0, K= 0			
2	1072	377	1056
4	2545	995	2530
* 6	5356	2956	5712
8	34	43	50
* 10	8626	4619	10183
12	874	287	934
H= 0, K= 2			
2	62	46	47
4	1061	25	1064
6	131	116	142
8	929	243	873
10	1862	1233	1832
12	21	1	2
H= 0, K= 4			
2	103	30	47
4	922	186	862
6	164	127	181
8	529	146	457
10	849	594	865
12	5	7	24
H= 0, K= 6			
* 0	21551	12448	24896
2	81	36	36
4	275	45	114
6	925	411	952
8	692	457	582
10	3629	1583	3624
12	59	0	137
H= 0, K= 8			
2	72	66	74
4	329	76	261
6	161	10	35
8	673	170	691
10	1587	1012	1559
12	38	6	9
H= 0, K= 10			
0	0	134	269
2	121	16	71
4	175	41	239
6	62	10	19
8	35	2	20
10	78	43	44
12	0	19	25
H= 0, K= 12			
0	1363	1276	2553
2	310	205	318
4	0	3	18
6	2	1	12
8	434	265	304
10	355	176	431
H= 0, K= 14			
0	294	301	602
2	307	148	332
4	1297	632	1228
6	121	64	157
8	1888	749	1830
10	191	65	99
H= 0, K= 16			
* 0	280	362	725
2	13	0	22
4	93	37	165
6	24	5	30
8	0	12	23
10	294	56	272
H= 0, K= 18			
0	89	31	63
2	160	72	98
4	0	40	40
6	41	2	4
8	78	2	14
H= 0, K= 20			
0	134	355	711
2	107	4	8
4	31	50	80
6	75	7	10
H= 1, K= 1			
1	1448	702	1409
* 3	16171	9875	19762
5	3892	1784	3744
7	787	65	258
9	1171	550	1145
11	4	9	40
13	1031	664	1107
H= 1, K= 3			
1	0	0	0
3	93	15	72
5	12	5	6
7	267	143	206
9	14	0	8
11	0	0	0
13	0	7	11
H= 1, K= 5			
1	144	35	140
3	6436	3330	6471
5	771	251	720
7	1258	588	1249
9	45	7	94
11	101	90	97
13	208	118	236
H= 1, K= 7			
1	244	113	160
* 3	8766	4113	8944
5	1534	763	1495
7	689	118	656
9	360	192	409
11	64	0	1
H= 1, K= 9			
1	491	239	508
3	283	271	351
5	533	328	507
7	249	186	200
9	84	57	64
11	32	23	49
H= 1, K= 11			
1	254	48	302
3	1008	728	1186
5	121	33	204
7	51	19	131
9	8	2	63
11	0	14	27
H= 1, K= 13			
1	484	199	522
3	130	48	188
5	63	0	0
7	1888	600	1829
9	143	23	34
11	168	90	158
H= 1, K= 15			
1	190	57	130
3	775	408	674
5	243	191	304
7	269	281	344
9	0	2	5
H= 1, K= 17			
1	41	9	38
3	74	2	10
5	20	25	25
7	0	42	57
9	55	8	4
H= 1, K= 19			
1	8	1	3
3	0	14	42
5	183	16	48
7	239	73	272
H= 1, K= 21			
1	129	70	129
3	860	386	758
H= 1, K= 23			
1	21	2	17
3	269	11	19
H= 2, K= 0			
0	1075	678	1056
* 2	6602	4731	8059
* 4	6396	4095	6908
* 6	17875	12376	26367
8	1890	825	1987
10	782	498	663
12	251	63	252
H= 2, K= 2			
0	87	1	47
* 2	4853	3351	5198
4	257	7	192
6	2343	1494	2353
8	35	6	8
10	106	22	40
12	65	38	38
H= 2, K= 4			
0	90	17	47
2	3274	2172	3366
4	73	100	114
6	1031	733	1032
8	38	4	22
10	189	69	132
12	58	2	4
H= 2, K= 6			
0	155	1	35
2	1323	594	1033
4	1807	900	1542
* 6	10330	4944	10483
8	172	14	155
10	38	44	51
12	74	21	27
H= 2, K= 8			
0	78	7	74
2	1411	846	1422
4	1398	572	1225
6	1962	1106	1939
8	60	56	58
10	0	15	15
12	43	19	20
H= 2, K= 10			
0	123	55	71
2	303	162	305
4	46	85	85
6	0	2	53
8	21	12	38
10	82	3	124
12	0	1	1
H= 2, K= 12			
0	334	113	318
2	188	20	27
4	83	39	138
6	1531	771	1578
8	68	85	92
10	0	5	43
H= 2, K= 14			
0	313	184	332
2	1802	769	1872
4	130	70	113
6	82	39	53
8	314	63	270
10	159	49	146

Table 5 (*cont.*)

	L	F^2o	F^2c	$F^2c(S)$
H= 2, K= 16				
	0	23	22	22
	2	39	0	45
	4	175	140	181
	6	917	287	909
	8	0	32	35
	10	100	1	160
H= 2, K= 18				
	0	156	26	93
	2	21	4	20
	4	0	0	37
	6	77	80	121
	8	73	18	39
H= 2, K= 20				
	0	84	4	8
	2	303	47	164
	4	452	182	344
	6	373	121	289
H= 2, K= 22				
	0	33	24	25
	2	61	28	28
	4	211	70	89
H= 3, K= 1				
	1	49	19	26
	3	76	14	21
	5	3100	1308	3029
	7	101	33	107
*	9	10767	6572	12381
	11	584	273	634
	13	135	17	105
H= 3, K= 3				
	1	245	24	211
	3	115	40	152
	5	73	8	21
	7	0	1	7
	9	169	15	35
	11	53	1	17
	13	0	0	13
H= 3, K= 5				
	1	556	44	390
	3	293	27	346
	5	159	33	164
	7	124	114	121
*	9	4569	2450	4608
	11	36	2	76
H= 3, K= 7				
	1	1138	741	1009
	3	318	161	235
	5	1685	710	1790
	7	70	0	1
*	9	6654	3683	6813
	11	99	72	134
H= 3, K= 9				
	1	257	0	212
	3	19	4	25
	5	307	131	215
	7	75	79	87
	9	944	399	955
	11	7	11	11
H= 3, K= 11				
	1	55	65	86
	3	84	34	65
	5	186	19	95
	7	0	19	55
	9	796	367	654
	11	8	29	54
H= 3, K= 13				
	1	2886	1809	3005
	3	1588	760	1606
	5	13	5	8
	7	292	170	284
	9	892	489	853
	11	178	43	82
H= 3, K= 15				
	1	546	137	456
	3	165	98	137
	5	281	95	173
	7	0	0	30
	9	1101	398	970
H= 3, K= 17				
	1	11	15	24
	3	20	15	18
	5	44	3	3
	7	0	4	23
	9	87	3	58
H= 3, K= 19				
	1	249	230	415
	3	237	48	158
	5	0	7	17
	7	15	5	6
H= 3, K= 21				
	1	85	51	111
	3	34	13	13
	5	293	96	223
H= 3, K= 23				
	1	86	43	149
	3	23	38	62
H= 4, K= 0				
	0	2566	1535	2530
*	2	14897	11871	19770
*	4	6411	3618	6884
	6	363	67	292
*	8	5480	3009	5665
	10	1073	378	1145
	12	3699	2275	3791
H= 4, K= 2				
	0	1075	814	1064
	2	690	38	593
	4	438	298	479
	6	983	494	892
	8	209	31	209
	10	235	102	239
	12	664	393	694
H= 4, K= 4				
	0	912	677	862
	2	832	115	720
	4	431	340	480
	6	215	96	176
	8	0	51	97
	10	0	18	26
	12	246	178	302
H= 4, K= 6				
	0	264	69	114
	2	5573	3351	5313
	4	1673	801	1519
	6	1750	632	1810
	8	1796	865	1768
	10	258	32	253
	12	1251	731	1169
H= 4, K= 8				
	0	328	185	261
	2	604	67	377
	4	135	25	84
	6	628	404	746
	8	660	249	583
	10	622	358	65
	12	555	287	519
H= 4, K= 10				
	0	190	198	239
	2	521	63	235
	4	148	104	203
	6	80	71	77
	8	92	162	162
	10	0	81	91
H= 4, K= 12				
	0	0	14	18
	2	3	65	83
	4	158	26	126
	6	1325	414	1277
	8	291	106	369
	10	165	1	133
H= 4, K= 14				
	0	1257	596	1228
	2	62	64	120
	4	683	218	660
	6	1910	952	1917
	8	26	5	6
	10	36	22	25
H= 4, K= 16				
	0	190	129	165
	2	31	6	15
	4	254	51	189
	6	214	163	169
	8	338	137	201
H= 4, K= 18				
	0	0	0	40
	2	88	18	35
	4	179	0	55
	6	102	18	96
	8	145	37	133
H= 4, K= 20				
	0	25	30	80
	2	0	22	28
	4	0	0	14
	6	223	152	342
H= 4, K= 22				
	0	62	13	14
	2	202	1	6
H= 5, K= 1				
	1	708	258	660
	3	906	360	863
	5	6396	3209	6324
	7	107	48	101
	9	43	41	58
	11	671	289	677
H= 5, K= 3				
	1	117	20	108
	3	40	4	6
	5	62	17	30
	7	144	21	133
	9	45	9	19
	11	0	7	8
H= 5, K= 5				
	1	183	11	139
	3	47	0	5
	5	2341	1387	2354
	7	132	50	62
	9	118	36	106
	11	32	7	81
H= 5, K= 7				
	1	265	28	300
	3	239	87	311
	5	1466	695	1531
	7	82	33	57
	9	0	6	21
	11	310	95	241
H= 5, K= 9				
	1	79	31	31
	3	446	293	374
	5	129	11	53
	7	126	2	125
	9	47	2	8
	11	51	77	92
H= 5, K= 11				
	1	8	31	34
	3	117	11	48
	5	415	277	403
	7	38	0	17
	9	0	0	43
H= 5, K= 13				
	1	450	257	392
	3	146	89	112
	5	135	50	106
	7	1079	500	876
	9	300	67	256
H= 5, K= 15				
	1	42	0	1
	3	95	97	107
	5	0	1	11
	7	148	50	210
	9	0	49	49
H= 5, K= 17				
	1	0	24	26
	3	0	4	11
	5	40	0	38
	7	62	0	13
H= 5, K= 19				
	1	0	10	27
	3	0	3	11
	5	76	0	11
H= 5, K= 21				
	1	0	7	32
	3	167	83	119
H= 6, K= 0				
*	0	5407	2756	5712
*	2	4593	3652	5451
	4	6512	3409	6257
	6	222	151	170
*	8	7309	4967	8519
	10	245	136	241
	12	55	6	87
H= 6, K= 2				
	0	26	150	142
	2	40	25	40
	4	339	49	437
	6	1076	836	1050
	8	1779	751	1660
	10	43	19	20
	12	194	55	107
H= 6, K= 4				
	0	157	54	181
	2	53	39	44
	4	77	15	78
	6	974	885	1001
	8	870	439	868
	10	20	22	56
H= 6, K= 6				
	0	1117	540	952
	2	1342	1039	1281
	4	1470	873	1461
	6	113	19	105
	8	2809	1691	2767
	10	24	14	21
H= 6, K= 8				
	0	148	24	35
	2	102	9	114
	4	1648	489	1568
	6	367	280	396
	8	1227	653	1286
	10	69	26	43
H= 6, K= 10				
	0	0	10	19
	2	104	32	137
	4	0	38	40
	6	154	238	239
	8	99	34	36
	10	0	5	34
H= 6, K= 12				
	0	7	11	12
	2	153	188	194
	4	85	98	130
	6	40	57	80
	8	251	156	258
	10	140	92	110
H= 6, K= 14				
	0	140	93	157
	2	163	78	141
	4	212	57	171
	6	1078	450	1000
	8	112	26	34
H= 6. K= 16				
	0	16	25	30
	2	357	86	355
	4	289	63	158
	6	2	10	16
H= 6, K= 18				
	0	51	2	4
	2	0	57	69
	4	44	31	41
	6	0	1	20
H= 6, K= 20				
	0	127	3	10
	2	125	19	26
	4	297	124	203
H= 7, K= 1				
	1	7723	3968	7827
*	3	5015	2535	5201
	5	90	57	81
	7	2857	1362	2873
	9	113	3	101
	11	642	486	726
H= 7, K= 3				
	1	51	20	29
	3	31	38	38
	5	54	20	47
	7	53	24	25
	9	23	19	20
	11	62	12	17
H= 7, K= 5				
	1	2743	1290	2770
	3	1247	797	1299
	5	79	0	131
	7	388	197	458
	9	116	94	100
	11	92	131	160
H= 7, K= 7				
	1	2536	1320	2556
	3	2843	1250	2797
	5	82	19	42
	7	1868	915	1944
	9	4	0	55
H= 7, K= 9				
	1	134	31	57
	3	77	583	879
	5	38	1	1
	7	444	333	481
	9	90	146	171
H= 7, K= 11				
	1	467	133	420
	3	334	248	360
	5	0	37	113
	7	176	28	92
	9	33	15	19
H= 7, K= 15				
	1	19	1	1
	3	203	49	158
	5	641	284	647
	7	162	112	223
	9	117	42	50
H= 7, K= 15				
	1	24	32	36
	3	642	351	586
	5	17	42	49
	7	411	155	245
H= 7, K= 17				
	1	62	42	42
	3	0	1	2
	5	12	15	56
H= 7, K= 19				
	1	53	0	6
	3	324	41	155
H= 8, K= 0				
	0	62	7	50
	2	544	240	565
*	4	9294	6566	10616
	6	3118	1930	3118
	8	1696	1229	1742
	10	1124	617	1020
H= 8, K= 2				
	0	911	630	873
	2	283	168	230
	4	886	81	837
	6	461	95	394
	8	117	13	148
	10	178	36	167
H= 8, K= 4				
	0	537	311	457
	2	274	262	316
	4	452	38	477
	6	138	1	181
	8	69	3	17
	10	43	6	49
H= 8, K= 6				
	0	722	123	582
	2	56	13	15
	4	3448	2222	3397
	6	768	509	734
	8	333	378	415
	10	187	131	189
H= 8, K= 8				
	0	658	521	691
	2	0	5	13
	4	514	52	559
	6	559	224	512
	8	194	83	281
	10	245	98	237
H= 8, K= 10				
	0	30	18	20
	2	25	122	134
	4	18	20	46
	6	27	21	45
	8	0	6	59
H= 8, K= 12				
	0	430	40	306
	2	86	72	83
	4	325	161	260
	6	41	37	87
	8	26	80	82
H= 8, K= 14				
	0	1888	1081	1830
	2	248	135	241
	4	78	43	49
	6	80	0	3
H= 8, K= 16				
	0	15	11	23
	2	0	58	75
	4	282	150	231
	6	183	62	91
H= 8, K= 18				
	0	0	11	14
	2	49	9	37
	4	64	1	17
H= 9, K= 1				
	1	176	158	221
	3	162	62	202
	5	546	369	509
*	7	5263	2951	5723
	9	1122	487	1090
H= 9, K= 3				
	1	6	40	53
	3	39	1	10
	5	52	3	75
	7	97	8	13
	9	36	5	5
H= 9, K= 5				
	1	0	46	124
	3	149	18	64
	5	1081	643	1060
	7	2000	1233	2111
	9	201	65	196
H= 9, K= 7				
	1	43	7	16
	3	22	2	53
	5	652	492	650
	7	2647	1218	2761
*	9	237	196	459
H= 9, K= 9				
	1	33	13	16
	3	0	17	20
	5	114	1	155
	7	369	216	406
H= 9, K= 11				
	1	0	133	195
	3	0	2	16
	5	93	121	130
	7	354	160	292
H= 9, K= 13				
	1	749	242	592
	3	172	98	167
	5	1047	653	946
	7	253	75	223
H= 9, K= 15				
	1	25	40	45
	3	51	13	27
	5	288	60	395
H= 9, K= 17				
	1	0	42	71
	3	27	7	9
H= 10, K= 0				
*	0	8480	5564	10183
	2	5690	3613	5921
	4	95	2	140
	6	729	615	817
	8	41	2	10
H= 10, K= 2				
	0	1858	399	1832
	2	752	157	776
	4	413	341	468
	6	65	2	85
	8	111	81	84
H= 10, K= 4				
	0	822	272	865
	2	97	5	102
	4	70	33	94
	6	0	57	85
	8	145	259	259
H= 10, K= 6				
	0	3607	2041	3624
	2	2185	1577	2208
	4	733	103	763
	6	45	122	125
	8	83	78	100
H= 10, K= 8				
	0	1611	546	1559
	2	1228	342	1233
	4	691	492	693
	6	79	19	103
	8	32	2	17
H= 10, K= 10				
	0	75	1	44
	2	104	38	62
	4	0	39	49
	6	52	45	47
H= 10, K= 12				
	0	370	255	431
	2	392	450	532
	4	618	71	580
	6	0	21	21
H= 10, K= 14				
	2	176	20	144
	4	1487	775	1450
H= 11, K= 1				
	1	140	352	948
	3	4369	2116	4580
	5	1194	603	1174
	7	34	39	55
H= 11, K= 3				
	1	12	16	17
	3	35	1	4
	5	15	3	3
	7	3	9	11
H= 11, K= 5				
	1	16	5	17
	3	1468	840	1506
	5	157	169	219
	7	14	4	3
H= 11, K= 7				
	1	813	222	837
	3	2017	768	2092
	5	528	262	528
H= 11, K= 9				
	1	262	270	349
	3	213	131	249
	5	143	67	108
H= 11, K= 11				
	1	0	4	17
	3	130	108	173
	5	82	68	73
H= 11, K= 13				
	1	20	8	105
	3	136	16	95
H= 12, K= 0				
	0	930	647	934
	2	937	718	1109
	4	98	49	83
*	6	6253	3760	6687
H= 12, K= 2				
	0	29	1	2
	2	198	31	242
	4	21	41	59
	6	1243	476	1329
H= 12, K= 4				
	0	18	17	24
	2	6	13	26
	4	108	165	165
H= 12, K= 6				
	0	92	137	157
	2	249	217	267
	4	10	4	9
H= 12, K= 8				
	0	46	2	9
	2	413	149	459
	4	62	1	50
H= 12, K= 10				
	0	0	6	25
	2	0	52	68
H= 13, K= 1				
	1	1135	558	1154
	3	15	0	14
H= 13, K= 3				
	1	28	5	13
	3	78	33	48
H= 13, K= 5				
	1	101	158	216
H= -1, K= 1				
	1	1477	707	1409
	3	45	7	26
	5	728	403	660
*	7	7547	3858	7827
	9	201	64	221
	11	967	596	948
	13	1123	596	1154
H= -1, K= 3				
	1	0	0	0
	3	230	188	211
	5	244	88	108
	7	55	9	29
	9	34	12	54
	11	19	1	17
	13	0	8	13
H= -1, K= 5				
	1	148	105	140
	3	568	345	390
	5	221	129	139
	7	2773	1480	2770
	9	0	78	124
	11	28	13	17
	13	179	58	216
H= -1, K= 7				
	1	224	47	160
	3	1105	263	1008
	5	262	272	300
	7	2621	1237	2556
	9	49	9	16
	11	838	616	837
H= -1, K= 9				
	1	528	269	508
	3	255	211	212
	5	110	1	31
	7	174	27	57
	9	25	4	16
	11	257	74	349
H= -1, K= 11				
	1	261	254	302
	3	56	22	86
	5	0	3	34
	7	414	287	420
	11	28	14	17
H= -1, K= 13				
	1	490	323	522
	3	2946	1196	3005
	5	468	135	392
	7	3	0	1
	9	749	350	592
	11	48	97	105
H= -1, K= 15				
	1	78	73	130
	3	510	319	458
	5	40	0	1
	7	0	4	36
	9	19	6	45
H= -1, K= 17				
	1	33	30	38
	3	2	9	24
	5	0	1	26
	7	86	0	42
	9	0	29	71
H= -1, K= 19				
	1	25	2	3
	3	211	185	415
	5	0	17	27
	7	40	6	6
H= -1, K= 21				
	1	156	6	129
	3	44	60	111
	5	71	25	32
H= -1, K= 23				
	1	14	15	17
	3	79	105	149
H= -2, K= 0				
	0	939	678	1056
*	2	6119	3328	8059
*	4	14366	7899	19770
*	6	4337	1798	5451
	8	540	324	565
	10	5904	2309	5921
	12	930	391	1109
H= -2, K= 2				
	0	68	1	47
*	2	4864	1847	5198
	4	690	555	593
	6	79	24	49
	8	174	62	230
	10	803	619	776
	12	196	211	242
H= -2, K= 4				
	0	79	17	47
	2	3311	1194	3366
	4	815	600	720
	6	33	5	44
	8	276	54	316
	10	111	97	102
	12	30	13	26
H= -2, K= 6				
	0	99	1	36
	2	1095	438	1962
*	4	5153	1962	5313
	6	1204	242	1281
	8	82	2	15
	10	2279	632	2203
	12	222	51	267
H= -2, K= 8				
	0	76	7	74
	2	1413	576	1422
	4	615	311	3077
	6	95	105	114
	8	4	8	13
	10	1243	892	1233
	12	369	310	459
H= -2, K= 10				
	0	100	55	71
	2	350	144	305
	4	545	166	235
	6	86	99	131
	8	18	12	134
	10	135	24	62
	12	29	14	66
H= -2, K= 12				
	0	330	113	318
	2	177	7	27
	4	28	18	88
	6	160	7	194
	8	49	13	85
	10	388	81	532
H= -2, K= 14				
	0	308	184	332
	2	1718	1103	1872
	4	15	57	120
	6	156	64	141
	8	219	107	241
	10	109	90	110
H= -2, K= 16				
	0	0	22	22
	2	68	45	45
	4	65	8	15
	6	315	269	355
	8	0	16	75
H= -2, K= 18				
	0	143	26	98
	2	40	17	20
	4	57	18	35
	6	46	12	64
	8	62	27	37
H= -2, K= 20				
	0	120	4	8
	2	287	116	164
	4	0	6	28
	6	85	7	26
H= -2, K= 22				
	0	0	24	25
	2	7	0	28
	4	187	5	6
H= -2, K= 24				
	0	104	0	5
H= -3, K= 1				
*	1	15791	9887	19762
	3	9	7	21
	5	886	503	863
*	7	5015	2665	5201
	9	167	144	202
	11	4462	2465	4580
	13	42	14	14
H= -3, K= 3				
	1	106	57	74
	3	150	113	152
	5	26	1	6
	7	57	1	38
	9	37	8	10
	11	69	3	4
	13	76	16	48
H= -3, K= 5				
*	1	6236	2941	6471
	3	426	318	346
	5	37	5	5
	7	1223	502	1299
	9	120	46	64
	11	1503	666	1506
H= -3, K= 7				
	1	9055	4831	8944
	3	328	75	235
	5	235	224	311
	7	2851	1547	2797
	9	31	54	56
	11	2052	1325	2092
H= -3, K= 9				
	1	294	80	351
	3	23	21	25
	5	451	80	374
	7	766	293	879
	9	0	3	20
	11	199	118	249
H= -3, K= 11				
	1	1107	458	1186
	3	51	31	65
	5	89	37	48
	7	285	112	360
	9	33	14	16
	11	272	65	173
H= -3, K= 13				
	1	114	140	188
	3	1636	846	1606
	5	110	23	112
	7	150	109	158
	9	193	69	167
	11	157	79	95
H= -3, K= 15				
	1	750	266	674
	3	149	39	137
	5	111	10	107
	7	656	235	586
	9	58	14	27
H= -3, K= 17				
	1	174	8	10
	3	0	3	10
	5	0	1	2
	9	8	2	9
H= -3, K= 19				
	1	0	28	42
	3	173	110	158
	5	0	7	11
	7	347	114	155
H= -3, K= 21				
	1	834	372	158
	3	27	1	13
	5	167	36	119
H= -3, K= 23				
	1	263	8	19
	3	27	24	62
H= -4, K= 0				
	0	2424	1534	2530
*	2	6244	2812	6908
*	4	6047	3266	6884
	6	6210	2843	6257
*	8	9297	4049	10615
	10	114	138	140
	12	129	35	83
H= -4, K= 2				
	0	1845	814	1064
	2	264	186	192
	4	469	182	479
	6	347	388	437
	8	868	757	837
	10	404	122	463
	12	25	18	57
H= -4, K= 4				
	0	900	677	862
	2	75	13	114
	4	480	140	480
	6	62	61	78
	8	453	440	477
	10	51	42	74
	12	115	0	165
H= -4, K= 6				
	0	249	69	114
	2	1630	643	1542
	4	1602	718	1519
	6	1588	587	1461
	8	3319	1175	3397
	10	833	660	763
	12	71	5	9
H= -4, K= 8				
	0	291	185	261
	2	1449	654	1225
	4	140	59	84
	6	1727	1080	1568
	8	532	507	559
	10	713	201	693
	12	39	50	50
H= -4, K= 10				
	0	174	198	239
	2	135	0	82
	4	171	99	203
	6	0	2	40
	8	47	27	46
	10	0	10	49
H= -4, K= 12				
	0	0	14	18
	2	102	99	138
	4	0	100	126
	6	90	31	130
	8	255	99	260
	10	595	508	588
H= -4, K= 14				
	0	1300	598	1228
	2	114	43	113
	4	680	442	660
	6	249	114	171
	8	14	6	49
	10	1443	678	1450
H= -4, K= 16				
	0	151	129	165
	2	209	42	181
	4	143	138	189
	6	288	96	158
	8	250	87	231
H= -4, K= 18				
	2	0	36	37
	4	181	55	55
	6	45	10	41
	8	0	16	17
H= -4, K= 20				
	0	52	30	80
	2	477	162	344
	4	0	14	14
	6	245	85	208
H= -4, K= 22				
	0	35	13	14
	2	226	19	89
	4	101	19	26
H= -5, K= 1				
	1	3873	1960	3744
	3	3140	1720	3029
*	5	6094	3114	6324
	7	81	24	81
	9	515	139	509
	11	1258	569	1174
H= -5, K= 3				
	1	10	1	8
	3	37	13	21
	5	113	13	30
	7	74	27	47
	9	55	72	75
	11	0	0	3
H= -5, K= 5				
	1	783	469	720
	3	156	131	164
	5	2354	967	2354
	7	40	131	131
	9	1136	418	1060
	11	155	50	219
H= -5, K= 7				
	1	1546	732	1495
	3	1731	1088	1798
	5	1510	838	1531
	7	73	23	42
	9	648	158	650
	11	534	267	528
H= -5, K= 9				
	1	506	179	507
	3	306	84	215
	5	84	42	53
	7	36	0	1
	9	97	154	155
	11	120	41	108
H= -5, K= 11				
	1	187	171	204
	3	87	75	95
	5	387	126	400
	7	0	76	113
	9	103	9	130
	11	73	3	73
H= -5, K= 13				
	1	21	0	0
	3	0	3	8
	5	129	56	106
	7	608	363	647
	9	1029	313	946
H= -5, K= 15				
	1	285	112	304
	3	261	77	173
	5	0	10	11
	7	35	7	49
	9	262	335	396
H= -5, K= 17				
	1	64	0	25
	3	4	0	3
	5	43	38	38
	7	62	42	56
H= 05, K= 19				
	1	139	32	48
	3	0	10	17
	5	22	11	11
H= -5, K= 21				
	1	371	171	394
	3	275	127	223
H= -6, K= 0				
*	0	5282	2756	5712
*	2	17991	14023	26399
	4	319	225	292
	6	228	19	170
	8	3168	1188	3118
	10	773	202	817
	12	6628	2926	6657
H= -6, K= 2				
	0	130	26	142
	2	2527	860	2353
	4	1010	398	892
	6	1143	214	1050
	8	418	299	394
	10	62	82	85
	12	1250	853	1329
H= -6, K= 4				
	0	173	54	181
	2	1092	299	1032
	4	195	80	176
	6	977	116	1001
	8	115	182	183
	10	38	28	85
H= -6, K= 6				
	0	996	540	952
*	2	8999	5539	10483
	4	1817	1178	1810
	6	102	86	105
	8	776	226	734
	10	44	2	125
H= -6, K= 8				
	0	116	24	35
	2	1983	833	1939
	4	817	342	746
	6	408	115	396
	8	530	288	512
	10	112	84	103
H= -6, K= 10				
	0	0	10	19
	2	42	51	53
	4	62	6	77
	6	176	1	239
	8	38	24	45
	10	13	2	47
H= -6, K= 12				
	0	22	11	12
	2	1498	808	1578
	4	1306	865	1277
	6	123	23	80
	8	19	50	87
	10	40	0	21
H= -6, K= 14				
	0	121	93	157
	2	65	14	53
	4	1945	906	1917
	6	1065	551	1000
	8	78	3	3
H= -6, K= 16				
	0	14	25	30
	2	956	622	909
	4	203	4	169
	6	8	6	16
	8	144	29	91
H= -6, K= 18				
	0	73	2	4
	2	58	41	121
	4	71	78	96
	6	0	19	20
H= -6, K= 20				
	0	79	3	10
	2	285	88	209
	4	173	190	342
H= -7, K= 1				
	1	283	193	258
	3	101	75	107
	5	132	60	101
	7	2913	1510	2873
	9	5720	2778	5728
	11	24	15	55
H= -7, K= 3				
	1	248	63	206
	3	0	7	7
	5	138	112	133
	7	5	1	25
	9	63	5	13
	11	54	3	11
H= -7, K= 5				
	1	1320	662	1242
	3	123	7	121
	5	132	12	62
	7	45	261	458
	9	2090	878	2111
	11	11	59	63
H= -7, K= 7				
	1	678	538	656
	3	54	1	1
	5	54	24	57
	7	1898	1033	1948
	9	2705	1543	2761
H= -7, K= 9				
	1	238	14	200
	3	56	8	87
	5	132	123	125
	7	456	148	481
	9	398	190	406
H= -7, K= 11				
	1	71	111	131
	3	9	36	55
	5	43	11	17
	7	131	64	92
	9	321	131	292
H= -7, K= 13				
	1	1914	1229	1829
	3	310	114	284
	5	1020	377	876
	7	140	110	223
	9	311	148	223
H= -7, K= 15				
	1	274	62	344
	3	36	30	30
	5	198	166	216
	7	376	90	245
H= -7, K= 17				
	1	37	15	57
	3	0	21	23
	5	94	13	13
H= -7, K= 19				
	1	197	199	272
	3	65	1	6
H= -8, K= 0				
	0	6	7	50
	2	1960	1162	1987
	4	5643	2645	5655
*	6	7801	3552	8519
	8	1806	514	1742
	10	32	7	10
H= -8, K= 2				
	0	925	630	873
	2	86	1	8
	4	160	178	209
	6	1800	908	1168
	8	92	134	148
	10	63	4	84
H= -8, K= 4				
	0	527	311	457
	2	33	18	22
	4	0	46	97
	6	888	427	866
	8	47	14	17
	10	134	0	259
H= -8, K= 6				
	0	711	125	582
	2	197	141	155
	4	1877	903	1768
	6	2885	1076	2767
	8	400	37	418
	10	67	22	100
H= -8, K= 8				
	0	660	521	691
	2	35	1	58
	4	679	334	583
	6	1311	733	1286
	8	234	198	281
	10	33	15	17
H= -8, K= 10				
	0	30	18	20
	2	0	26	38
	4	110	0	162
	6	95	2	36
	8	4	53	59
H= -8, K= 12				
	0	417	40	304
	2	91	7	92
	4	279	263	369
	6	264	102	258
	8	0	1	82
H= -8, K= 14				
	0	1875	1081	1830
	2	283	207	270
	4	36	2	6
	6	50	3	34
H= -8, K= 16				
	0	0	11	23
	2	0	2	35
	4	295	64	201
	6	234	213	251
H= -8, K= 18				
	0	44	11	14
	2	45	21	39
	4	105	96	133
H= -9, K= 1				
	1	1163	595	1145
*	3	11010	5810	12581
	5	32	17	53
	7	125	97	101
	9	1118	602	1090
H= -9, K= 3				
	1	0	3	8
	3	69	20	35
	5	27	11	19
	7	18	0	20
	9	5	0	5
H= -9, K= 5				
	1	43	87	94
	3	4688	2158	4608
	5	153	69	106
	7	84	7	10
	9	180	132	196
H= -9, K= 7				
	1	378	217	400
	3	6801	3130	6813
	5	0	14	21
	7	20	55	55
	9	466	262	459
H= -9, K= 9				
	1	118	7	64
	3	969	556	955
	5	37	6	8
	7	67	25	177
H= -9, K= 11				
	1	6	61	63
	3	785	287	654
	5	7	42	43
	7	46	3	19
H= -9, K= 13				
	1	188	10	34
	3	908	364	853
	5	254	189	256
	7	86	8	50
H= -9, K= 15				
	1	0	3	5
	3	1019	572	970
	5	0	0	49
H= -9, K= 17				
	1	28	0	4
	3	45	54	58
H= -10, K= 0				
*	0	8760	5564	10185
	2	765	167	665
	4	1160	768	1145
	6	254	105	241
	8	1210	403	1020
H= -10, K= 2				
	0	1891	599	1832
	2	115	18	40
	4	239	136	239
	6	42	1	20
	8	111	131	167
H= -10, K= 4				
	0	852	272	865
	2	182	64	132
	4	9	3	26
	6	5	35	56
	8	9	43	49
H= -10, K= 6				
	0	3705	2041	3624
	2	18	7	51
	4	261	221	253
	6	19	7	21
	8	238	58	189
H= -10, K= 8				
	0	1581	546	1559
	2	0	0	15
	4	621	298	658
	6	83	17	43
	8	25	139	237
H= -10, K= 10				
	0	100	1	44
	2	117	121	124
	4	67	10	91
	6	7	29	34
H= -10, K= 12				
	0	404	255	431
	2	0	38	43
	4	121	131	133
	6	143	18	110
H= -10, K= 14				
	0	144	35	99
	2	138	98	146
	4	0	2	25
H= -10, K= 16				
	0	286	216	272
	2	110	159	160
H= -11, K= 1				
	1	21	31	40
	3	634	361	634
	5	749	388	677
	7	713	24	726
H= -11, K= 3				
	1	20	0	0
	3	39	16	17
	5	0	0	8
	7	14	5	17
H= -11, K= 5				
	1	122	8	97
	3	36	74	76
	5	49	74	81
	7	97	29	160
H= -11, K= 7				
	1	14	0	1
	3	105	62	134
	5	308	145	241
H= -11, K= 9				
	1	37	26	49
	3	0	0	11
	5	6	16	92
H= -11, K= 11				
	1	24	13	27
	3	41	26	54
	5	42	38	34
H= -11, K= 13				
	1	183	69	158
	3	151	35	82
H= -12, K= 0				
	0	850	647	934
	2	248	189	252
	4	3968	1516	3791
	6	58	31	87
H= -12, K= 2				
	0	46	1	2
	2	26	0	38
	4	603	301	694
	6	175	52	107
H= -12, K= 4				
	0	7	17	24
	2	15	2	4
	4	269	124	302
H= -12, K= 6				
	0	80	137	137
	2	56	6	27
	4	1226	438	1169
H= -12, K= 8				
	0	28	2	9
	2	45	1	20
	4	555	232	519
H= -12, K= 10				
	0	0	0	25
	2	5	1	1
H= -13, K= 1				
	1	1045	444	1107
	3	120	89	105
H= -13, K= 3				
	1	49	3	11
	3	19	13	13
H= -13, K= 5				
	1	169	118	236

Mössbauer studies of Hazony, Earl & Lefkowitz (1967) have indicated that the water molecules, K^+ ions, and $Fe(CN)_6^{4-}$ ions all contribute to the ferroelectric mechanism.

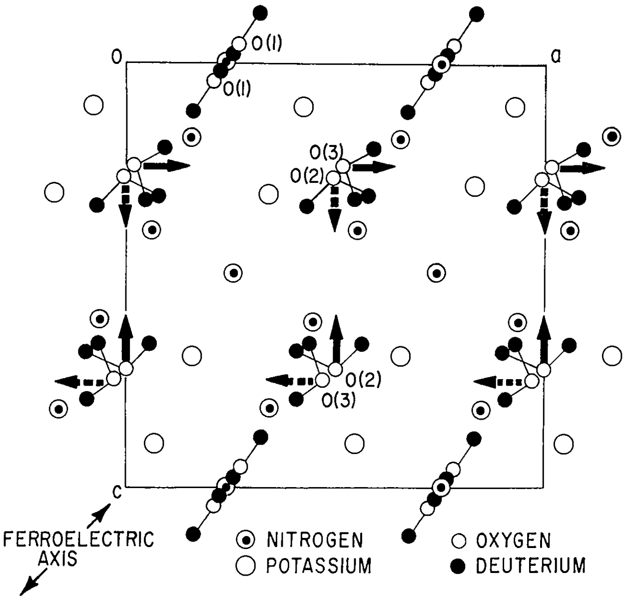


Fig. 6. KFCT water molecule layer at $y=0{\cdot}5$ showing the ferroelectric axis. Water dipoles associated with one ferroelectric state are marked by the solid arrows, and with the other state by dotted arrows.

Further elucidation of the complex behavior of KFCT below the Curie temperature can best be obtained by a series of neutron diffraction studies at lower temperatures with an electrical field first along [$\bar{1}$01] and then a reversed field. This type of investigation was made by Bacon & Pease (1955) on KH_2PO_4 and would also allow a check on possible movements of the K^+ and the ferrocyanide ions.

We wish to thank Dr Y. Baskin for the optical measurements, Dr L. Heaton and Mr H. Knott for helpful discussions, and Mr J. Gvildys and Dr. G. W. Cox for considerable assistance in programming. We are indebted to Dr D. E. O'Reilly for analysis of the deuterated crystals and for stimulating discussions.

References

Bacon, G. E. & Pease, R. S. (1955). *Proc. Roy. Soc.* A**230**, 359.

Blinc, R., Brenman, M. & Waugh, J. S. (1961). *J. Chem. Phys.* **35**, 1770.

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *ORFLS, A Fortran Crystallographic Least-Squares Program.* Oak Ridge National Laboratory Rept. ORNL-TM-305.

Cochran, W. (1960). *Advanc. Phys.* **9**, 387.

Donnay, J. D. H. (1963). *Crystal Data*, 2nd ed. ACA Monograph, No. 5.

Evans, H. T. (1961). *Acta Cryst.* **14**, 689.

Hazony, Y., Earls, D. & Lefkowitz, I. (1968). *Phys. Rev.* **166**, 507.

Kennicott, P. R. (1963). General Electric Research Laboratory, Rept. No. 63-RL-(33216).

Kiriyama, R., Kiriyama, H., Wada, T., Niizeki, N. & Hirabayashi, H. (1964). *J. Phys. Soc. Japan*, **19**, 540.

Mueller, M. H., Heaton, L. & Miller, K. T. (1960). *Acta Cryst.* **13**, 828.

O'Reilly, D. E. & Tsang, T. (1967). *J. Chem. Phys.* **47**, 4072.

Pospelov, V. A. & Zhdanov, G. S. (1947*a*). *Zh. Fiz. Khim.* **21**, 405.

Pospelov, V. A. & Zhdanov, G. S. (1947*b*). *Zh. Fiz. Khim.* **21**, 879.

Toyoda, H., Niizeki, N. & Waku, S. (1960). *J. Phys. Soc. Japan*, **15**, 1831.

Tsang, T. & O'Reilly, D. E. (1965). *J. Chem. Phys.* **43**, 4234.

Waku, S., Hirabayashi, H., Toyoda, H. & Iwasaki, H. (1959). *J. Phys. Soc. Japan*, **14**, 973.

Waku, S., Masuro, K. & Tanaka, T. (1959). *J. Phys. Soc. Japan*, **15**, 1968.

Waku, S., Masuro, K., Tanaka, T. & Iwasaki, H. (1960). *J. Phys. Soc. Japan*, **15**, 1185.

Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1970). A26, 567

Arcing and polytypism.

By V. K. Agrawal, *Department of Physics, Hastinapur College (University of Delhi), Moti Bagh, New Delhi-23, India*

(*Received* 12 *February* 1970)

An X-ray study of the arcing phenomenon in polytypic crystals of CdI_2, PbI_2 and $CdBr_2$ has revealed that various polytypes are formed by the creation of stacking faults at different regular intervals during crystal growth.

An X-ray study of a large number of crystals of three polytypic substances, *viz.* 120 of CdI_2 (Agrawal & Trigunayat, 1969*a,b*), 60 of PbI_2 (Agrawal, Chadha & Trigunayat, 1970*a*) and 12 of $CdBr_2$ (Agrawal & Trigunayat, 1970), has revealed that the arcing phenomenon, which consists of an extension of the diffraction spots into small