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CRYSTAL AND MAGNETIC STRUCTURE OF $KFeO_2$

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Abstract—The crystal and magnetic structures of $KFeO_2$ have been determined by neutron and X-ray powder-diffraction and Mössbauer-effect techniques. The crystal structure at 4.2 K and 300 K is orthorhombic and the magnetic space group is *Pbca′*. The Fe^{3+}-ions in this structure are tetrahedrally coordinated by oxygen ions, and each Fe^{3+}-ion has a magnetic moment which is antiferromagnetically coupled to the moments of four Fe^{3+}-neighbours. The direction of the moments is parallel to the *a*-axis. A crystal phase transition has been observed near the Néel temperature–960 K.

INTRODUCTION

The crystal structure of $KFeO_2$ has been the subject of few publications. According to the first model [1] it is face centered cubic with $a_{cub} = 7.958$ Å, closely related to β-cristobalite. It was then shown that the structure was not exactly face centered cubic and the space group was determined to be T^4 [2]. Additional information was that $KFeO_2$ crystallizes in the form of regular octahedrons (but not larger than 30 μ) and that its density is 3.38 g/cm³ [3]. Because of difficulties in growing single crystal and the hygroscopic nature of this compound a more precise study has been impossible.

Vielhaber and Hoppe [4] indicated a whole group of compounds that should crystallize with the same structure which was determined using a single crystal of $KGaO_2$. This structure is orthorhombic and the space group is D_{2h}^{15}-*Pbca*. The unit cell contains 16 formula units with lattice constants

$$a \approx a_{cub}/\sqrt{2}, \quad b \approx a_{cub}\sqrt{2}, \quad c \approx 2a_{cub}.$$

These lattice constants were recently confirmed in the case of $KFeO_2$ [5].

The essential feature of this structure is the existence of infinite $Me^{3+}O_4^{2-}$ chains of tetrahedra running in different directions with the monovalent atoms located in large spaces in between. The tetrahedrons have a corner in common.

The magnetic data for $KFeO_2$ have up to now been derived mainly from Mössbauer effect data. Ichida *et al.* [6] determined, from the temperature dependence of the internal magnetic field, the magnetic transition temperature T_N to be 983 ± 10 K. This dependence follows the Brillouin function for the spin value $S = 5/2$. The Mössbauer spectrum at 993 K did not show quadrupole splitting. They also stated on the basis of magnetic susceptibility measurements that $KFeO_2$ is a compensated antiferromagnetic, but no anomaly has been observed near T_N in the susceptibility-temperature curve. The value of T_N for $KFeO_2$ is among the highest Néel temperatures for all iron compounds.

The present investigation was undertaken in order to determine the crystal structure of $KFeO_2$ and its magnetic ordering scheme.

PREPARATION AND MEASUREMENTS

The $KFeO_2$ sample was prepared in the following way: A mixture of α-Fe_2O_3 and K_2CO_3 (with a small excess of K_2CO_3) made into tablets was heated at 800°C for 2 hr. The product was crushed and heated again in the form of tablets at 800°C for 20 hr.

X-Ray powder diagrams were taken with a DRON-1 diffractometer (CoK_α radiation). Preliminary neutron diffraction data have been collected on the KSN diffractometer in the Boris Kidrič Institute, Yugoslavia in the temperature range 77–1000 K. At 4.2, 300 and 1000 K more precise measurements were carried out on the powder diffractometer with a neutron wavelength of 2.575 Å at the H.F.R. of Reactor Centrum Nederland, the Netherlands. The Mössbauer effect measurement was carried out at 300 K using a $^{57}Co(Cr)$ source.

CRYSTAL AND MAGNETIC STRUCTURE

The X-ray diagrams showed a number of very small peaks in addition to strong pseudocubic peaks. All peaks could be indexed by assuming an orthorhombic unit cell with lattice constants

$$a \approx a_{cub}/\sqrt{2}, \quad b \approx b_{cub}\sqrt{2}, \quad c \approx 2a_{cub}.$$

Several X-ray diffractograms were taken with increasing temperature. Around 980 K a small jump (0.5%) of the lattice constants was observed with a clear change of intensities of these small peaks.

Figure 1 shows the neutron diagrams taken at 300 and 1000 K (the diagram at 4.2 K is identical to that at 300 K). In the neutron diagram at 300 K a series of extra peaks is visible which could be indexed on the basis of the orthorhombic unit cell mentioned above.

Assuming the $KGaO_2$ type crystal structure at 300 K, all atoms occupy the following 8(*c*) general positions in the space group *Pbca*

$$x, y, z:\ 1/2 + x, 1/2 - y, \bar{z};$$
$$\bar{x}, \bar{y}, \bar{z}:\ 1/2 - x, 1/2 + y, z;$$
$$\bar{x}, 1/2 + y, 1/2 - z;\ 1/2 - x, \bar{y}, 1/2 + z;$$
$$x, 1/2 - y, 1/2 + z;\ 1/2 + x, y, 1/2 - z.$$

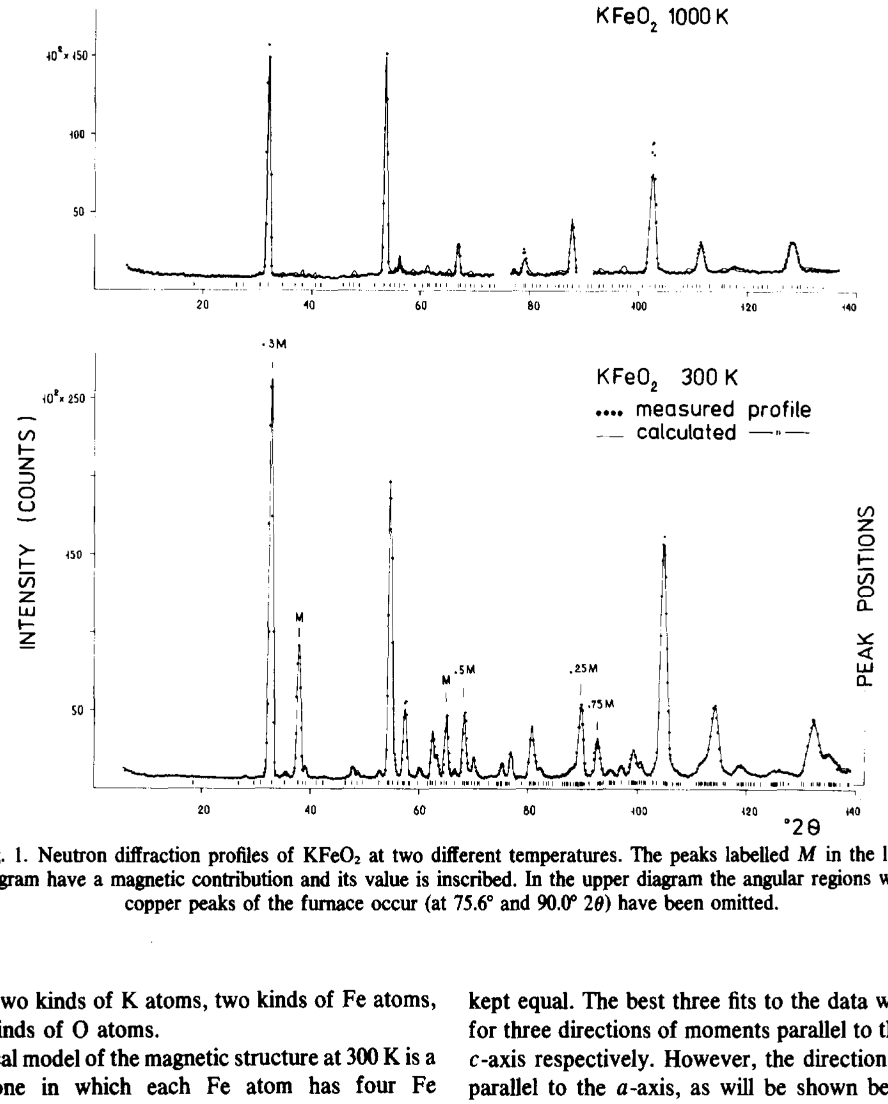

Fig. 1. Neutron diffraction profiles of $KFeO_2$ at two different temperatures. The peaks labelled M in the lower diagram have a magnetic contribution and its value is inscribed. In the upper diagram the angular regions where copper peaks of the furnace occur (at 75.6° and 90.0° 2θ) have been omitted.

There are two kinds of K atoms, two kinds of Fe atoms, and four kinds of O atoms.

The logical model of the magnetic structure at 300 K is a collinear one in which each Fe atom has four Fe neighbours having antiparallel moments coupled to it through the oxygen atoms. The signs of moments, if the Fe atoms are labelled in the sequence of the coordinates above, are (− + + − + − − +) for Fe(I) and with opposite signs for Fe(II). This configurational spin symmetry leads to the following form of the magnetic structure factor

$$F_{hkl} = 0.2695 \sin \eta f_{hkl}\left[-8 \sum_{n=1}^{2} \mu_n \cos 2\pi\left(hx_n - \frac{h-k}{4}\right) \times \cos 2\pi\left(ky_n - \frac{k-l}{4}\right) \sin 2\pi\left(lz_n - \frac{l-h}{4}\right)\right]$$

where h, k, l are the Miller indices of the reflections; x_n, y_n, z_n are the atomic positions of two kinds of Fe atoms; μ_n are their magnetic moments in μ_B; η is the angle between the magnetic moment and the scattering vector and f_{hkl} is the magnetic form factor of the Fe moment.

The refinement of the crystallographic parameters and of the magnitude of the Fe moments was carried out by the profile method[7]. In this refinement an overall isotropic temperature factor and the spherical form factor for Fe^{3+} given by Watson and Freemen[8] were used. The magnetic moments of the two kinds of Fe atoms were kept equal. The best three fits to the data were obtained for three directions of moments parallel to the a-, b- and c-axis respectively. However, the direction of moments parallel to the a-axis, as will be shown below, is most probable. Assuming this direction, the compound may be assigned to the magnetic space group $Pbca'$.

The calculated and observed integrated intensities for $KFeO_2$ at 300 K are compared in Table 1. In the lower part of Fig. 1 the calculated and observed neutron diffraction profiles at 300 K are shown and the calculated magnetic contributions are marked. The final values for the parameters at 4.2 and 300 K are given in Table 2. The interatomic distances are given in Table 3.

Measurements of the magnetic intensity as a function of temperature were taken for the (004) + (120) peak at $2\theta = 37.6°$. The transition temperature deduced in this way is 960 ± 10 K as is seen from Fig. 2. The corresponding reduced magnetization was calculated and is compared in Fig. 3 with the Brillouin function for $S = 5/2$.

The structure refinement, based on the space group $Pbca$ at 1000 K, did not lead to satisfactory intensity agreement, as it can be seen from the upper part of Fig. 1. The diagram at 1000 K could not be indexed with a smaller unit cell. The unit cell may be either tetragonal with $a \approx b_{\text{orth}}$, $c \approx c_{\text{orth}}$ or cubic of $CsScO_2$ type[4] with $a = 16.160$ Å $\approx c_{\text{orth}}$.

The Mössbauer absorption spectrum taken at 300 K is

Table 1. Calculated (magnetic and total) and observed integrated intensities for $KFeO_2$ at 300 K

h	k	l	2θ	I_{mag}	I_{tot}	I_{obs}	h	k	l	2θ	I_{mag}	I_{tot}	I_{obs}
0	0	2	18.50	3	62	0	2	1	7	94.86	0	774	790
0	2	0	26.35	0	0	147	2	5	1	94.86	12	437	452
1	0	0	26.46	0	0	0	3	1	3	95.11	0	649	760
0	2	1	27.97	569	684	484	1	6	2	95.47	0	17	20
1	1	0	29.63	130	130	1000	3	3	2	95.87	2	239	178
1	1	1	31.10	0	60	912	2	2	6	97.09	59	3585	3559
0	2	2	32.40	32157	78658	79986	2	5	2	97.13	69	425	422
1	0	2	32.51	9268	55851	55716	0	6	4	98.42	0	182	164
1	1	2	35.21	179	783	1940	3	0	0	98.89	0	1785	1679
0	0	4	37.62	21663	21944	22906	0	2	9	99.14	24	322	304
1	2	0	37.69	20859	20859	21339	1	4	7	99.12	19	3697	3489
0	2	3	38.81	23	3801	3420	1	6	3	99.22	103	1624	1533
1	2	1	38.92	219	244	225	2	2	7	99.36	21	2564	2425
1	1	3	41.28	1	2	296	2	4	5	99.40	83	1440	1363
1	2	2	42.34	0	483	187	3	2	3	99.65	1	2973	2910
0	2	4	46.51	0	158	226	1	3	8	99.97	48	266	289
1	0	4	46.51	5	50	61	3	1	4	100.40	0	979	1239
1	2	3	47.63	68	3104	3602	3	3	0	100.40	42	42	54
1	1	4	48.64	0	2014	1501	1	1	9	100.73	0	744	946
1	3	0	48.64	134	134	100	2	5	3	100.91	2	2075	2513
1	3	1	49.61	2	303	633	3	3	1	101.16	1	654	713
1	3	2	52.49	112	1850	2319	1	5	6	103.03	23	1294	1434
0	4	0	54.29	0	26784	26524	3	3	2	103.46	45	2872	3034
1	2	4	54.36	104	47525	47138	0	4	8	104.51	44	17630	18359
2	0	0	54.54	0	25331	25076	1	6	4	104.58	18	51740	53715
0	2	5	55.19	3	5064	4516	2	0	8	104.72	29	18075	18654
0	4	1	55.22	111	1992	1775	3	2	4	105.01	5	42703	43608
2	1	0	56.38	0	2	4	0	6	5	105.30	5	3194	3252
1	1	5	57.06	1	6199	6765	1	2	9	105.30	27	2207	2247
1	3	3	57.06	6	7275	7944	2	1	8	106.27	1	4873	4835
2	1	1	57.24	0	9846	10897	2	5	4	106.27	109	164	162
0	0	6	57.89	2	149	152	2	3	7	107.06	4	1091	876
0	4	2	57.89	1	362	368	3	1	5	107.35	0	855	663
2	0	2	58.14	1	172	146	3	3	3	107.35	3	1467	1155
2	1	2	59.87	73	3253	2803	0	0	10	107.60	0	441	412
1	4	0	61.42	2	2	0	2	4	6	107.86	0	66	97
2	2	0	61.60	0	0	0	1	4	8	110.84	0	1194	1362
0	4	3	62.21	238	283	262	2	2	8	110.99	4	43	46
1	2	5	62.24	23	9579	8910	2	6	0	111.02	0	174	185
1	4	1	62.24	31	3616	3365	3	4	0	111.31	5	5	5
2	2	1	62.42	31	1075	1008	1	6	5	111.67	48	4090	4487
1	3	4	63.11	0	6711	6482	2	6	1	111.85	177	1013	1117
2	1	3	64.12	0	158	105	3	2	5	112.10	1	43	48
0	2	6	64.69	4280	4552	4481	3	4	1	112.10	3	1173	1289
1	0	6	64.73	5123	5174	5290	1	7	0	112.46	15	15	16
1	4	2	64.76	7598	7814	8080	3	3	4	112.93	0	7905	8334
2	2	2	64.94	2817	3341	3841	1	3	9	113.26	0	332	346
1	1	6	66.38	81	2475	1797	1	5	7	113.26	0	808	841
0	4	4	67.97	8803	11959	10990	1	7	1	113.29	1	487	507
2	0	4	68.18	2847	10213	10828	2	5	5	113.44	3	796	825
1	4	3	68.83	361	1177	1330	0	2	10	114.01	1537	8217	8415
2	2	3	68.98	4	776	840	0	6	6	114.01	841	8182	8377
2	1	4	69.77	208	1891	2052	1	0	10	114.05	736	9535	9761
2	3	0	69.80	0	4051	4407	2	6	2	114.26	1447	6181	6333
1	3	5	70.42	3	138	145	3	0	6	114.55	396	8936	9234
2	3	1	70.59	8	692	621	3	4	2	114.55	586	6114	6324
1	2	6	71.21	8	27	20	1	1	10	115.70	14	1204	1520
2	3	2	72.94	104	896	935	1	7	2	115.74	14	1245	1599
1	4	4	74.34	3	18	119	3	1	6	116.21	63	276	419
2	2	4	74.48	7	9	35	0	4	9	118.15	8	101	129
0	2	7	75.02	41	1497	1895	2	4	7	118.40	27	27	31
0	4	5	75.06	150	2771	3462	2	6	3	118.44	18	446	514
1	5	0	75.89	46	46	55	3	4	3	118.73	30	5001	5195
1	1	7	76.64	0	1461	1425	2	3	8	119.27	0	2227	2052
1	5	1	76.64	1	5384	5230	1	7	3	119.99	6	3049	3001
2	1	5	76.79	0	776	746	2	1	9	120.13	0	345	356
2	3	3	76.82	0	2065	1985	3	3	5	120.46	3	51	61
1	3	6	78.95	51	59	175	1	2	10	120.78	3	118	173
1	5	2	78.95	39	40	113	1	6	6	120.82	4	12	18
0	0	8	80.39	47	9273	9126	3	2	6	121.32	9	416	823

Table 1. (*Contd*)

h	k	l	2θ	I_{mag}	I_{tot}	I_{obs}	h	k	l	2θ	I_{mag}	I_{tot}	I_{obs}
2	4	0	80.64	0	10041	9883	2	5	6	122.76	39	126	330
1	2	7	81.22	46	3050	3158	2	6	4	124.60	7	827	1037
1	4	5	81.22	268	536	555	3	4	4	124.88	0	1030	1254
2	2	5	81.36	1	1351	1408	0	6	7	125.21	101	713	875
2	4	1	81.40	30	118	123	1	4	9	125.28	1	13	16
2	3	4	82.12	183	2999	3255	2	2	9	125.46	20	1353	1692
1	5	3	82.73	8	566	652	1	5	8	126.18	29	275	371
0	4	6	83.41	1	19	23	1	7	4	126.22	0	1210	1635
2	0	6	83.63	0	34	19	3	5	0	126.76	53	53	72
2	4	2	83.63	7	56	27	3	1	7	127.66	0	215	286
2	1	6	85.14	77	112	0	3	5	1	127.69	1	1918	2541
0	2	8	86.40	5	26	12	1	3	10	130.00	11	136	130
0	6	0	86.44	0	416	200	3	3	6	130.57	66	402	387
1	0	8	86.47	0	432	212	3	5	2	130.57	50	693	669
3	0	0	86.90	0	0	0	0	8	0	131.94	0	5821	6141
0	6	1	87.19	266	508	324	2	4	8	132.19	43	36182	37733
2	4	3	87.37	97	775	537	0	2	11	132.88	2	3243	4172
1	1	8	87.95	69	2581	2271	0	8	1	132.98	47	3252	3154
1	5	4	87.98	0	258	229	1	6	7	133.02	150	689	665
3	1	0	88.42	8	8	8	4	0	0	133.09	0	3037	2908
1	3	7	88.70	0	2263	2162	2	6	5	133.24	7	202	190
2	3	5	88.88	0	1082	1046	3	2	7	133.60	7	775	705
3	1	1	89.14	0	753	743	3	4	5	133.60	37	128	117
0	6	2	89.42	2018	10395	10380	2	7	0	134.28	0	579	500
1	4	6	89.46	4262	7689	7683	1	1	11	135.04	0	2179	1794
2	2	6	89.60	1831	5630	5633	1	7	5	135.11	4	402	329
3	0	2	88.89	88	9397	9398	4	1	0	135.18	0	9322	7580
3	1	2	91.40	21	121	175	2	3	9	135.29	3	2786	2232
1	2	8	92.45	6741	8340	7532	2	5	7	135.32	9	3553	2838
1	6	0	92.48	3055	3055	2782	2	7	1	135.36	18	734	584
2	4	4	92.63	4105	4466	4262	3	5	3	135.72	12	258	191
3	2	0	92.88	323	323	338	0	4	10	136.04	1	172	115
0	4	7	93.13	39	2536	2776	0	8	2	136.12	1	766	500
0	6	3	93.17	20	57	63	4	1	1	136.22	0	0	0
1	6	1	93.20	312	754	826	2	0	10	136.33	4	145	85
3	2	1	93.64	3	196	200	4	0	2	137.34	0	82	24
2	5	0	94.14	0	129	118	2	1	10	138.56	61	2917	303
1	5	5	94.72	5	679	648	2	7	2	138.64	40	353	35

$$R = 100\,\Sigma|I_{obs} - I_{tot}| \Big/ \sum I_{obs} = 6.1.$$

The calculated intensities are normalized to the observed intensities. The observed integrated intensities are separated according to the calculated values of the integrated intensities.

Table 2. Structural, magnetic and Mössbauer parameters in $KFeO_2$

Atom	x		y		z	
	4.2 K	300 K	4.2 K	300 K	4.2 K	300 K
8K(I)	0.758[7]	0.769[5]	0.008[3]	0.004[2]	0.072[3]	0.074[2]
8K(II)	0.816[3]	0.811[3]	0.262[3]	0.260[2]	0.180[2]	0.185[2]
8Fe(I)	0.243[2]	0.249[2]	0.006[2]	0.008[2]	0.183[1]	0.184[1]
8Fe(II)	0.285[1]	0.280[1]	0.263[1]	0.261[1]	0.065[1]	0.064[1]
8O(I)	0.591[1]	0.583[3]	0.289[2]	0.291[1]	0.017[1]	0.022[1]
8O(II)	0.157[4]	0.166[3]	0.416[2]	0.410[2]	0.096[1]	0.099[1]
8O(III)	0.282[3]	0.287[2]	0.169[2]	0.171[2]	0.161[1]	0.158[1]
8O(IV)	0.068[4]	0.089[4]	0.481[1]	0.481[1]	0.284[1]	0.282[1]

$\mu_{Fe}(\mu_B)$		a(Å)		b(Å)		c(Å)	
4.2 K	300 K	4.2 K	300 K	4.2 K	300 K	4.2 K	300 K
3.99[3]	3.81[3]	5.577[1]	5.600[1]	11.227[1]	11.249[1]	15.890[2]	15.914[2]

Temperature (K)	*IS* (mm/sec)	ϵ (mm/sec)	*H* (kOe)
300	$+0.152 \pm 0.015$	$+0.037 \pm 0.015$	501 ± 5

The errors in brackets are standard deviations based on statistics only. *IS*, isomer shift relative to metallic iron; ϵ, quadrupole interaction energy; *H*, internal magnetic field at the iron nuclei.

Table 3. Interatomic distances (in Å) and bond angles Fe–O–Fe in $KFeO_2$ at 300 K

Fe(I)–O	Fe(II)–O	K(I)–O	K(II)–O	Fe(I)–Fe(I)	Fe(I)–O(III)–Fe(II)
1.81	1.86	3.50	2.91	3.50[2×]	136.1°
1.90	1.86	3.56	3.13	Fe(II)–Fe(II)	Fe(I)–O(II)–Fe(II)
1.82	1.88	2.66	2.69	3.48[2×]	132.7°
1.99	1.80	2.69	2.84	Fe(I)–Fe(II)	Fe(I)–O(IV)–Fe(I)
O–O	K–K	2.44	2.95	3.43	132.8·[2×]
2.96	3.38	3.28	2.87	3.38	Fe(II)–O(I)–Fe(II)
2.92	3.29	2.98	3.32	Fe–K	138.9°[2×]
2.99	3.50	3.36	3.23	3.21	
2.98	3.48[2×]			3.25	

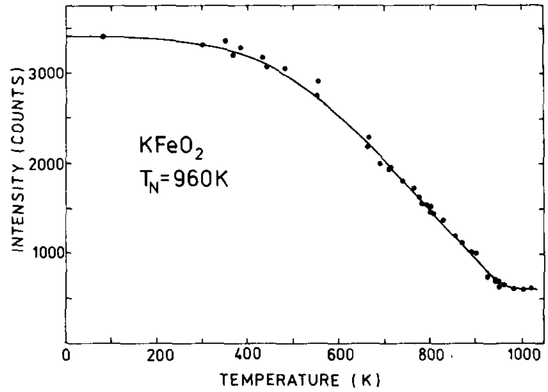

Fig. 2. Temperature dependence of the intensity of the magnetic peak at $2\theta = 37.6°$.

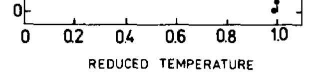

Fig. 3. Reduced temperature dependence of the sublattice magnetization of $KFeO_2$ derived from Fig. 2. The dots are the observed data, the full line is the Brillouin function for $S = 5/2$.

shown in Fig. 4. The spectrum was fitted assuming Lorentzian shaped lines. The Mössbauer parameters obtained are given in Table 2. It is seen that in the sample there exists one specified value 501 kOe of the internal magnetic field because the half width of the spectrum is rather small (0.40 mm/sec). This is in agreement with the assumption that the magnetic moments of two kinds of Fe atoms are equal.

The isomer shift (relative to metallic iron) is +0.152 mm/sec in agreement with the value +0.16 ± 0.03 mm/sec stated by Kerler *et al.*[9]. This value is typical for iron in the trivalent state. Because two pairs of internal absorption lines have a common centre, the quadrupole interaction energy ϵ can be determined as +0.037 mm/sec, (the value of Kerler *et al.* is +0.04 ± 0.012 mm/sec).

This value of ϵ may be compared with those calculated by means of a point charge model. For this purpose the electric field gradient tensor was calculated by summation in a sphere of 120 Å radius for Fe(I) and Fe(II) separately. All sums were well convergent. The structural parameters at 300 K were taken from three fits mentioned above. Then, by diagonalizing the Hamiltonian matrix in the case of simultaneous magnetic and electric interaction, the energy sublevels of the first excited nuclear state ($I = 3/2$) of ^{57}Fe were found. The quadrupole moment $Q = +0.20b$ for this state and the Sternheimer antishielding factor $(1 - \gamma_\infty) = 10.14$ for the Fe^{3+} ion were used. The calculated quadrupole interaction energies are given in Table 4. These values are equal for all crystallographically equivalent Fe ions and refer to their effective charge $Z = 3$. The absolute values at 300 K decrease with decreasing Z but the signs remain unchanged.

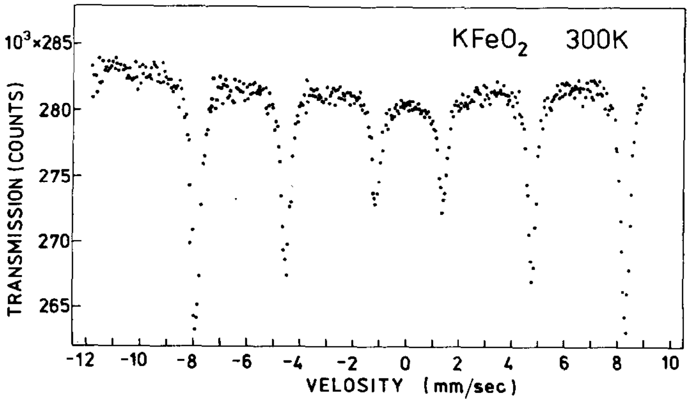

Fig. 4. Mössbauer absorption spectrum of $KFeO_2$ at 300 K. The velocity scale is relative to metallic iron.

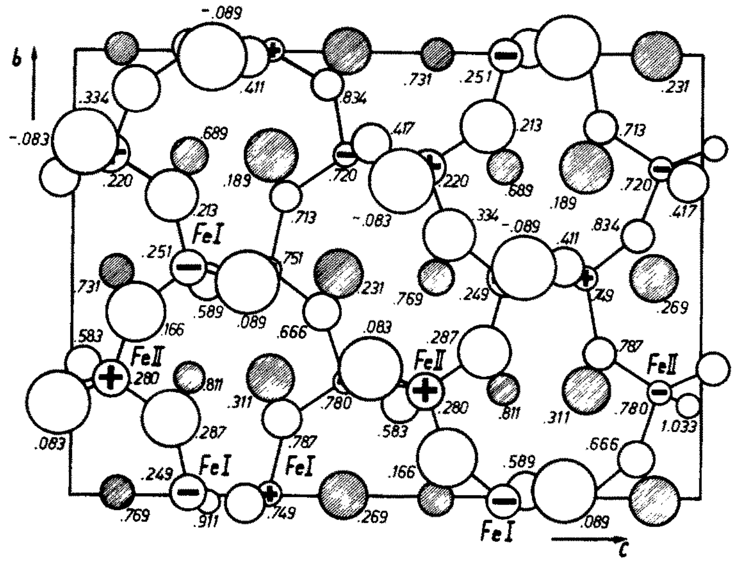

Fig. 5. Crystal and magnetic structure of $KFeO_2$ projected on the *bc*-plane. Open circles denote O atoms, hatched circles *K* atoms. The circles with + or − inside denote Fe atoms with spin parallel or antiparallel respectively to the *a*-axis. The numbers and the different sizes of circles indicate the vertical height of the different portions.

Table 4. Electric quadrupole ϵ and magnetic dipolar interaction energies *D* in $KFeO_2$ calculated for the different spin directions ($S = 5/2$)

		4.2 K		300 K	
		Fe(I)	Fe(II)	Fe(I)	Fe(II)
ϵ (mm/sec)	S‖a	+0.002	+0.02	+0.27	+0.08
	S‖b			−0.05	+0.15
	S‖c			−0.24	−0.22
2*D* (10^5 erg/cm^3)	S‖a	−1.61	−1.22	−1.13	−1.16
	S‖b	+1.44	+1.54	+1.14	+1.29
	S‖c	+0.16	−0.32	−0.01	−0.13

It is seen that only the spin direction along the *a*-axis gives the proper sign. The high value of ϵ for Fe(I) could be caused by neglecting the electric dipole contribution and by inaccuracies in the structural parameters obtained from powder measurements.

In $KFeO_2$ the magnetic dipolar interactions are the important source of the anisotropy. The dipolar energy *D* was computed by summation in a sphere of radius 120 Å. The structural parameters from Table 1 were used. The results are given in Table 4. It is seen that the value of *D* is smallest for the spins parallel to the *a*-axis.

DISCUSSION

The crystallographic structure of $KFeO_2$ is isotypic to that reported by Vielhaber and Hoppe for $KGaO_2$. Figure 5 presents the crystal and magnetic structure of $KFeO_2$ projected on the *bc*-plane.

The magnetic structure is similar to that in β-$NaFeO_2$[10]. In both compounds Fe atoms are in the centre of oxygen tetrahedrons, which have a corner in common, so that superexchange interaction should be responsible for the antiparallel coupling of magnetic moments. The distances Fe–O in both compounds are short (about 1.85 Å), and the distances Fe–K (3.21 Å) and Fe–Na (3.17 Å) are about equal in magnitude. The angles of the Fe–O–Fe bond in β-$NaFeO_2$ are 124° and 129°, somewhat smaller than in $KFeO_2$ (Table 3). However, the Néel temperature in β-$NaFeO_2$ is 723 K while in $KFeO_2$ it is about 960 K. The short Fe–O distances can cause covalency effects which reduce the value of the magnetic moment ($3.99\mu_B$ at 4.2 K).

The direction of spins parallel to the *a*-axis seems to be a logical one. If one takes another nearly cubic unit cell with $a = \sqrt{2}a_{\text{orth}} = 15.840(2)$ Å, $b = \sqrt{2}b_{\text{orth}} = 15.909(2)$ Å, $c = c_{\text{orth}} = 15.914(2)$ Å at 300 K, a distinct shortening of the *a*-axis becomes visible. The structure refinements with other directions of spins gave the same relations between the lattice constants. For comparison, in $KGaO_2$ which is nonmagnetic, $a = 15.59_9$ Å, $b = 15.66_4$ Å and $c = 15.81_8$ Å.

A change of crystal structure near T_N was observed. The structure above T_N should be more regular. This is in agreement with the fact that the Mössbauer spectrum shows no quadrupole splitting above T_N. In order to determine this structure a study of $KFeO_2$ with the use of single crystals is needed.

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