

Table 48A-2-001. $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$. Solubility A in water [62Kab].

A [wt%]	T [°C]	A [wt%]	T [°C]
1.25	−0.24	26.0	30
4.0	−0.62	27.8	35
8.0	−1.09	32.6	50
11.6	−1.6	36.8	65
12.5	0	38.2	70
15.0	5	40.1	80
17.4	10	41.34	87.3
19.3	15	41.99	94
22.0	20	42.63	99.6
24.0	25	44.77	104.1

Table 48A-2-002. $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$. Atomic coordinates at RT (in phase I) [64Kir].

Atom	Equivalent positions	x	y	z
Fe	4e	0.000	0.179	0.250
K (1)	8f	0.188	0.850	0.156
K (2)	8f	0.095	0.646	0.444
C (1)	8f	0.190	0.179	0.314
C (2)	8f	0.067	0.179	0.055
C (3)	4e	0.000	0.052	0.250
C (4)	4e	0.000	0.303	0.250
N (1)	8f	0.301	0.179	0.353
N (2)	8f	0.095	0.179	0.937
N (3)	4e	0.000	0.003	0.250
N (4)	4e	0.000	0.354	0.250
O (1)	4e	0.000	0.467	0.750
O (2)	8f	0.250	0.500	0.000

Table 48A-2-003. $K_4Fe(CN)_6 \cdot 3D_2O$. Atomic coordinates and temperature factors [70Tay]. b_{ij} is defined by Eq. (b) in Introduction. Water II is associated with O(2) and O(3) in general positions. See Fig. 48A-2-003.

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

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.

Table 48A-2-004. $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{H}_2\text{O}$. Refractive indices and optical axial angle [62Kay].

λ [nm]	n_α	n_β	n_γ	$2V$	Ref.
589	—	1.5772	—	$-78^\circ 10'$	1895Duf
486	1.582	1.587	1.594		65Bal
520	1.576	1.581	1.587		
555	1.573	1.578	1.583		
589	1.570	1.575	1.580		
620	1.567	1.572	1.577		
656	1.564	1.569	1.574		

Table 48A-2-005. $\text{K}_4\text{Fe}(\text{CN})_6 \cdot 3\text{D}_2\text{O}$. e^2qQ/h , η and directions of the principal axes at -73°C [65Tsa]. A, B, C and D are assigned to four pairs of lines. η : asymmetry parameter. The θ and ϕ_z are spherical coordinate angles when taking $X \parallel [101]$ and $Z \parallel [010]$.

	A	B	C	D
e^2qQ/h [kHz]	$-126 (1)$	$-126 (1)$	$-123 (2)$	$-123 (2)$
η	$0.96 (10)$	$0.96 (10)$	$0.63 (2)$	$0.63 (2)$
X direction θ	$37 (1)^\circ$	$37 (1)^\circ$	$70 (1)^\circ$	$70 (1)^\circ$
ϕ_z	$78 (9)^\circ$	$- 3 (6)^\circ$	$50 (3)^\circ$	$- 40 (3)^\circ$
Y direction θ	$127 (1)^\circ$	$127 (1)^\circ$	$81 (2)^\circ$	$81 (2)^\circ$
ϕ_z	$88 (3)^\circ$	$- 5 (3)^\circ$	$144 (2)^\circ$	$54 (2)^\circ$