

Table M21-001. KSCN. Unit cell parameters at several temperatures in phase I and phase II [87Yam2].

Tetragonal phase					
<i>T</i> [K]	415	417.5	424	435	
<i>a</i> [Å]	6.740(1)	6.741(1)	6.742(1)	6.746(1)	
<i>c</i> [Å]	7.832(3)	7.835(2)	7.843(2)	7.859(3)	

Orthorhombic phase					
<i>T</i> [K]	288	363	388	398	408
<i>a</i> [Å]	6.691(2)	6.715(1)	6.722(1)	6.725(2)	6.731(2)
<i>b</i> [Å]	6.676(2)	6.699(2)	6.709(2)	6.712(2)	6.720(2)
<i>c</i> [Å]	7.606(2)	7.684(2)	7.718(2)	7.738(2)	7.770(2)

Table M21-002. KSCN. Fractional coordinates and temperature parameters in phase I [87Yam2]. $b_{ij} [\cdot 10^{-4} \text{ Å}^2]$ is defined by Eq. (b) in Introduction.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>b</i> ₁₁	<i>b</i> ₂₂	<i>b</i> ₃₃	<i>b</i> ₁₂	<i>b</i> ₁₃	<i>b</i> ₂₃
435 K									
K	0	0	0.25	358(3)	358(3)	191(1)	0	0	0
S	0.6460(3)	0.1460(3)	0	196(3)	196(3)	234(2)	−17(2)	0	0
N	0.3560(8)	−0.1441(8)	0	156(9)	156(9)	332(11)	−40(6)	0	0
C	0.4739(9)	−0.0262(9)	0	159(17)	159(17)	209(7)	−6(8)	0	0
424 K									
K	0	0	0.25	352(3)	352(3)	185(1)	0	0	0
S	0.6460(3)	0.1460(3)	0	189(3)	189(3)	231(3)	−19(2)	0	0
N	0.3558(7)	−0.1443(7)	0	150(9)	150(9)	300(11)	−33(6)	0	0
C	0.4738(9)	−0.0261(9)	0	157(17)	157(17)	200(7)	−2(9)	0	0
417.5 K									
K	0	0	0.25	353(3)	353(3)	187(1)	0	0	0
S	0.6460(3)	0.1460(3)	0	187(3)	187(3)	229(2)	−20(2)	0	0
N	0.3561(8)	−0.1440(8)	0	153(8)	153(8)	313(10)	−26(6)	0	0
C	0.4735(8)	−0.0265(8)	0	155(16)	155(16)	204(7)	−4(8)	0	0
415 K									
K	0	0	0.25	348(3)	348(3)	179(1)	0	0	0
S	0.6461(3)	0.1461(3)	0	181(3)	181(3)	224(2)	−19(2)	0	0
N	0.3558(8)	−0.1443(3)	0	152(9)	152(9)	293(10)	−29(6)	0	0
C	0.4738(9)	−0.262(9)	0	152(16)	152(16)	195(7)	−1(8)	0	0

M21 KSCN, Potassium thiocyanate

Table M21-003. KSCN. Fractional coordinates and temperature parameters in phase II determined by X-ray diffraction [87Yam2]. The atoms in SCN^- with smaller occupancy are denoted as S' , C' and N' . b_{ij} [10^{-4} \AA^2] and B [\AA^2] are, respectively, defined by Eq. (b) and Eq. (e) in Introduction.

	x	y	z	b_{11} or B	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
408 K									
K	0.7789(1)	0.25	0	266(2)	274(2)	160(1)	0	0	−6(1)
S	0.3953(1)	0.1071(1)	0.25	155(2)	156(2)	228(2)	13(2)	0	0
N	0.1089(4)	0.4065(5)	0.25	130(6)	168(7)	278(8)	45(6)	0	0
C	0.2276(5)	0.2813(5)	0.25	145(6)	157(8)	175(7)	1(6)	0	0
S'	0.1034(10)	0.3951(10)	0.25	3.8(1)					
N'	0.3941(31)	0.1047(31)	0.25	3.5(3)					
C'	0.2822(28)	0.2304(30)	0.25	2.4(3)					
398 K									
K	0.7845(1)	0.25	0	240(2)	233(2)	149(1)	0	0	−8(1)
S	0.3952(1)	0.1074(1)	0.25	146(1)	144(1)	217(2)	15(1)	0	0
N	0.1134(4)	0.4097(4)	0.25	139(5)	174(6)	277(7)	41(5)	0	0
C	0.2285(4)	0.2840(4)	0.25	132(5)	142(6)	164(5)	0(4)	0	0
S'	0.0991(14)	0.3953(14)	0.25	3.4(1)					
N'	0.4000(35)	0.1042(34)	0.25	2.2(3)					
C'	0.2808(38)	0.2407(41)	0.25	2.2(4)					
388 K									
K	0.7866(1)	0.25	0	224(1)	211(1)	142(1)	0	0	−8(1)
S	0.3955(1)	0.1080(1)	0.25	139(1)	139(1)	209(2)	13(1)	0	0
N	0.1110(4)	0.4101(4)	0.25	135(5)	190(6)	250(6)	40(5)	0	0
C	0.2292(4)	0.2858(4)	0.25	131(5)	129(5)	154(5)	−4(4)	0	0
S'	0.0988(21)	0.3984(21)	0.25	3.2(2)					
N'	0.3890(54)	0.0864(52)	0.25	1.9(5)					
C'	0.2678(59)	0.2249(60)	0.25	1.9(6)					
363 K									
K	0.7891(1)	0.25	0	200(1)	186(1)	126(1)	0	0	−7(1)
S	0.3956(1)	0.1076(1)	0.25	130(1)	129(1)	191(1)	11(1)	0	0
N	0.1101(4)	0.4109(4)	0.25	131(4)	173(5)	210(5)	36(4)	0	0
C	0.2295(4)	0.2859(4)	0.25	122(4)	124(4)	140(4)	−7(3)	0	0
288 K									
K	0.7931(1)	0.25	0	147(1)	132(1)	91(1)	0	0	−5(1)
S	0.3963(1)	0.1078(1)	0.25	97(1)	95(1)	138(1)	8(1)	0	0
N	0.1113(4)	0.4162(4)	0.25	110(4)	130(4)	193(5)	24(4)	0	0
C	0.2306(3)	0.2881(3)	0.25	87(3)	87(3)	100(3)	−9(3)	0	0

Table M21-004. KSCN. Fractional coordinates and temperature parameters in phase II determined from neutron diffraction data [92Coo]. b_{ij} [\AA^2] is defined by Eq. (b) in Introduction.

Atom	x	b_{11}	y	b_{22}	z	b_{33}	b_{12}
K	0.2080(8)	0.0183(14)	0.25	0.0122(14)	0	0.0071(7)	0
S	0.6050(9)	0.0100(13)	0.1087(9)	0.0107(13)	0.25	0.0102(11)	0.0008(8)
C	0.7704(4)	0.0083(5)	0.2871(3)	0.0091(4)	0.25	0.0103(5)	0.0014(4)
N	0.8890(3)	0.0116(4)	0.4154(3)	0.0126(4)	0.25	0.0180(5)	0.0039(4)

Table M21-005. KSCN. Occupation probability of SCN ion in phase II [87Yam2].

T [K]	288	363	388	398	408
p_{SCN}	0.983(2)	0.988(2)	0.949(2)	0.918(2)	0.865(2)