

Table 39B-1-001. [(NH₄)_{1-x}K_x]₂SO₄. Fractional coordinates [$\cdot 10^{-4}$] and temperature parameters [$\cdot 10^{-4}$] [77Shi]. b_{ij} is defined by Eq. (b) in Introduction. $T = 293$ K.

Molar fraction = 0.31 ₄									
	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
N, K(1)	1831(4)	945(3)	2500	87(3)	48(2)	145(6)	5(2)	0	0
N, K(2)	4778(2)	7936(2)	2500	76(2)	50(1)	161(4)	-1(1)	0	0
S	2398(1)	4192(1)	2500	58(1)	37(1)	106(2)	-3(1)	0	0
O(1)	537(5)	3989(5)	2500	67(5)	125(6)	332(16)	-32(4)	0	0
O(2)	2793(6)	5574(3)	2500	139(7)	39(2)	250(12)	-15(3)	0	0
O(3)	3143(4)	3603(3)	464(5)	163(5)	80(3)	168(7)	19(3)	26(5)	-28(4)
Molar fraction = 0.70 ₀									
	x	y	z	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
N, K(1)	1775(1)	908(1)	2500	74(1)	41(1)	106(2)	0(1)	0	0
N, K(2)	4850(1)	7955(1)	2500	60(1)	38(0)	134(1)	-1(0)	0	0
S	2355(1)	4193(1)	2500	53(1)	25(0)	79(1)	-1(0)	0	0
O(1)	433(3)	4098(3)	2500	59(3)	84(3)	263(9)	-18(2)	0	0
O(2)	2902(4)	5592(2)	2500	115(4)	32(1)	172(6)	-14(2)	0	0
O(3)	3055(3)	3547(2)	421(3)	141(3)	56(1)	118(3)	16(2)	25(3)	-22(2)