

Table 39A-20-001. K₂ZnI₄. Fractional coordinates and isotropic temperature parameters in phase I [95Kas]. $T = 296$ K. Iodine atoms occupy two positions related by mirror reflections with equal probability. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å ²]
K(1)	0.0500(5)	0.25	0.7148(7)	5.01(15)
K(2)	0.5713(5)	0.25	0.7682(7)	5.24(16)
Zn	0.2023(2)	0.25	0.2820(3)	2.77(5)
I(1)	0.3711(2)	0.2228(4)	0.0801(2)	4.15(5)
I(2)	−0.0739(2)	0.2239(3)	0.1015(2)	3.92(5)
I(3)	0.2681(2)	0.5048(2)	0.4929(2)	3.22(4)
I(4)	0.2565(2)	0.0007(3)	0.5132(2)	3.24(4)

Table 39A-20-002. K₂ZnI₄. Interatomic distances [Å] and angles [°] in phase I [95Kas]. $T = 296$ K.

Zn–I(1)	2.605(3)	Zn–I(2)	2.608(2)
Zn–I(3)	2.592(2)	Zn–I(4)	2.647(2)
I(1)–Zn–I(2)	113.7(2)	I(1)–Zn–I(3)	111.8(1)
I(1)–Zn–I(4)	108.4(1)	I(2)–Zn–I(3)	114.2(1)
I(2)–Zn–I(4)	104.6(1)	I(3)–Zn–I(4)	103.1(2)

Table 39A-20-003. K₂ZnI₄. Fractional coordinates and isotropic temperature parameters in phase II [95Kas]. $T = 235$ K. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å ²]
K(1)	0.0509(5)	0.2767(11)	0.7179(7)	3.72(15)
K(2)	0.5699(6)	0.2794(11)	0.7657(8)	4.20(18)
Zn	0.2014(3)	0.25	0.2815(3)	2.28(5)
I(1)	0.3738(2)	0.2341(4)	0.0818(2)	4.22(5)
I(2)	−0.0763(2)	0.2296(4)	0.0997(2)	3.78(4)
I(3)	0.2562(2)	0.5141(3)	0.4859(2)	2.90(3)
I(4)	0.2654(2)	0.0095(3)	0.5182(2)	2.67(3)

Table 39A-20-004. K₂ZnI₄. Interatomic distances [Å] and angles [°] in phase II [95Kas]. $T = 235$ K.

Zn–I(1)	2.602(3)	Zn–I(2)	2.603(2)
Zn–I(3)	2.621(3)	Zn–I(4)	2.619(2)
I(1)–Zn–I(2)	114.1(2)	I(1)–Zn–I(3)	110.9(2)
I(1)–Zn–I(4)	109.2(2)	I(2)–Zn–I(3)	111.0(1)
I(2)–Zn–I(4)	108.0(1)	I(3)–Zn–I(4)	103.0(2)