

Table 39A-16-001. K₂ZnBr₄. Fractional coordinates and isotropic temperature parameters in phase I [94Mas]. $T = 564$ K. One of the two disordered configurations for Br atoms are listed. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B [Å ²]
K(1)	0.25	0.091(3)	0.129(3)	15.3(1)
K(2)	0.25	0.681(2)	0.990(3)	10.3(1)
Zn	0.25	0.421(1)	0.221(1)	6.2(1)
Br(1)	0.195(2)	0.428(1)	−0.024(1)	9.6(1)
Br(2)	0.307(2)	0.583(1)	0.323(1)	9.6(1)
Br(3)	0.481(3)	0.309(1)	0.285(2)	10.1(1)
Br(4)	−0.012(2)	0.361(1)	0.331(2)	8.7(1)

Table 39A-16-002. K₂ZnBr₄. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-2}$ Å²] in phase II [92Kas]. $T = 296$ K. Br atoms takes two configurations related by mirror reflection. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B
K(1)	439(4)	2500	7036(5)	508(10)
K(2)	5740(4)	2500	7802(5)	519(10)
Zn	2062(2)	2500	2814(2)	364(4)
Br(1)	3629(2)	2207(4)	738(2)	450(5)
Br(2)	−654(2)	2230(4)	1072(3)	476(5)
Br(3)	2666(3)	5008(3)	4985(3)	453(5)
Br(4)	2673(2)	−25(3)	5047(3)	415(5)

Table 39A-16-003. K₂ZnBr₄. Interatomic distances [Å] and angles [°] in phase II [92Kas]. $T = 296$ K.

Zn–Br(1)	2.401(11)	Zn–Br(2)	2.409(15)
Zn–Br(3)	2.406(5)	Zn–Br(3)	2.420(5)
Br(1)–Zn–Br(2)	113.3(3)	Br(1)–Zn–Br(3)	115.3(2)
Br(1)–Zn–Br(4)	106.3(2)	Br(2)–Zn–Br(3)	112.9(4)
Br(2)–Zn–Br(4)	104.8(4)	Br(3)–Zn–Br(4)	102.9(3)

Table 39A-16-004. K₂ZnBr₄. Fractional coordinates [$\cdot 10^{-4}$] and isotropic temperature parameters [$\cdot 10^{-2}$ Å²] in phase III [92Kas]. $T = 123$ K. B is defined by Eq. (e) in Introduction.

Atom	x	y	z	B
K(1)	488(4)	2761(7)	7097(6)	233(9)
K(2)	5712(4)	2771(8)	7743(6)	241(9)
Zn	2043(2)	2500	2797(3)	193(4)
Br(1)	3692(2)	2324(5)	786(3)	278(5)
Br(2)	−709(2)	2260(4)	1002(3)	267(5)
Br(3)	2584(2)	5116(3)	4843(3)	219(4)
Br(4)	2694(2)	67(3)	5163(3)	211(4)

Table 39A-16-005. K₂ZnBr₄. Interatomic distances [Å] and angles [°] in phase III [92Kas]. *T* = 123 K.

Zn–Br(1)	2.39(6)	Zn–Br(2)	2.41(9)
Zn–Br(3)	2.40(2)	Zn–Br(4)	2.43(3)
Br(1)–Zn–Br(2)	114(2)	Br(1)–Zn–Br(3)	112(1)
Br(1)–Zn–Br(4)	109(1)	Br(2)–Zn–Br(3)	111(2)
Br(2)–Zn–Br(4)	107(3)	Br(3)–Zn–Br(4)	102(1)