

**Table 25A-1-001.** KNiCl<sub>3</sub>. Structure [80Vis1].  $x, y, z$  at RT.

Atom	$x$	$y$	$z$
K	0.3353(2)	0.3353(2)	0.3294(6)
Ni(1)	0	0	0
Ni(2)	1/3	2/3	0.1230(1)
Cl(1)	0.1598(1)	0.20	0.2604(4)
Cl(2)	0.5056(1)	0.1732(1)	0.3852(2)

**Table 25A-1-002.** KNiCl<sub>3</sub>. Structure [80Vis1].  $U_{ij}$  [ $\text{\AA}^2$ ] at RT.  $U_{ij}$  is defined by Eq. (d) in Introduction.

Atom	$U_{11}$	$U_{22}$	$U_{33}$	$2U_{12}$	$2U_{23}$	$2U_{31}$
K	38(2)	38(2)	65(2)	41(8)	26(2)	26(2)
Ni(1)	21(1)	21(1)	17(1)	21(1)	0	0
Ni(2)	16(1)	16(1)	67(2)	16(1)	0	0
Cl(1)	23(2)	35(3)	27(2)	35(3)	0	-3(5)
Cl(2)	20(1)	21(1)	66(2)	7(2)	4(4)	2(4)