

Table 3. Fractional atomic coordinates, equivalent isotropic displacement parameters, occupancies, and atomic displacement parameters (\AA^2) for skutterudite and nickelskutterudite.

Element	x	y	z	U_{eq} (\AA^2)	Occ. (<1)	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
R050593											
M*	0.25	0.25	0.25	0.00310(18)	0.989(4)	0.00310(18)	0.00310(18)	0.00310(18)	0.00047(11)	0.00047(11)	0.00047 (11)
Fe	0	0	0	0.000(15)	0.0127(9)						
As	0.15012(4)	0.34300 (5)	0	0.00452(14)	0.967(5)	0.00434(17)	0.0057(2)	0.00350(16)	0.00054(10)	0	0
S	0.121(3)	0.273(4)	0	0.009(6)*	0.033(5)						
R100195											
Co	0.25	0.25	0.25	0.00227(13)	1.00(3)	0.00227(13)	0.00227(13)	0.00227(13)	0.00013(8)	0.00013(8)	0.00013 (8)
As	0	0.15024(2)	0.34280 (2)	0.00316(8)	0.99(3)	0.00211(10)	0.00295(11)	0.00442(11)	0	0	0.00048 (6)
R100194											
Ni1	0.25	0.25	0.25	0.00529(12)		0.00529(12)	0.00529(12)	0.00529(12)	0.00026(8)	0.00026(8)	0.00026 (8)
Ni2	0	0	0	0.01(3)	0.008(6)						
As	0	0.34685(2)	0.14960 (2)	0.00613(8)		0.00503(10)	0.00752(11)	0.00584(11)	0	0	0.00073 (6)
R100196											
M**	0.25	0.25	0.25	0.00471(15)		0.00471(15)	0.00471(15)	0.00471(15)	0.00023(11)	0.00023(11)	0.00023(11)
As**	0.14972(3)	0.34594(3)	0	0.00585(9)		0.00562(15)	0.00734(14)	0.00459(15)	0.00074(8)	0	0

Notes: *M = Co + Fe.

**M = $\text{Ni}_{0.59(5)}\text{Co}_{0.280(10)}\text{Fe}_{0.14(6)}$.

**As = $\text{As}_{0.99}\text{S}_{0.01}$.