Table 4. Selected interatomic distances and angles for nickelskutterudite R100196. The Ni, Co, and Fe site is identified as *M*. The theoretical icosahedral bond length, *A*-As, is included for purposes of discussion even though *A* is not occupied.

	Distance, Å		Angle (˚)
M—As	2.3634(2)	As^{i}—M—As	84.008(9)
As—As^{vii}	2.4749(5)	As^{i}—M—As^{ii}	95.992(9)
As—As^{viii}	2.5467(6)	As—M—As^{ii}	84.008(9)
		As^{i}—M—As^{iii}	84.008(9)
		As—M—As^{iii}	95.992(9)
		As^{ii}—M—As^{iii}	180.000(11)
		As^{iv}—M—As^{v}	84.007(9)
		M^{vi}—As—M	121.928(11)
		M^{vi}—As—As^{vii}	110.531(6)
		M^{vi}—As—As^{viii}	109.604(6)
		As^{vii}—As—As^{viii}	90.0