CuSe	*hP*156	(176) $P6_3/m$ – i^8h^8fedc

CuSe [1], klockmannite
Structural features: Close-packed Se layers in AABAAC stacking; Cu in (distorted) tetrahedral voids, and inside B- and C-stacked Se layers. One Se-Se dumbbell (parallel to [001]) for one single Se atom.

Lippmann F. (1962) [1]
CuSe
a = 1.42, c = 1.725 nm, c/a = 1.215, V = 3.0123 nm^3, Z = 78

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cu1	12*i*	1	0.02564	0.4359	0.107		tetrahedron Se_4
Se2	12*i*	1	0.07692	0.30769	0.066		tetrahedron $SeCu_3$
Se3	12*i*	1	0.15385	0.61538	0.066		tetrahedron $SeCu_3$
Cu4	12*i*	1	0.17949	0.05128	0.107		tetrahedron Se_4
Cu5	12*i*	1	0.25641	0.35897	0.107		tetrahedron Se_4
Se6	12*i*	1	0.30769	0.23077	0.066		tetrahedron $SeCu_3$
Cu7	12*i*	1	0.48718	0.28205	0.107		tetrahedron Se_4
Se8	12*i*	1	0.53846	0.15385	0.066		tetrahedron $SeCu_3$
Se9	6*h*	*m*..	0.02564	0.4359	$^1/_4$		trigonal bipyramid Cu_5
Cu10	6*h*	*m*..	0.12821	0.17949	$^1/_4$		coplanar triangle Se_3
Se11	6*h*	*m*..	0.17949	0.05128	$^1/_4$		trigonal bipyramid Cu_5
Cu12	6*h*	*m*..	0.20513	0.48718	$^1/_4$		coplanar triangle Se_3
Se13	6*h*	*m*..	0.25641	0.35897	$^1/_4$		trigonal bipyramid Cu_5
Cu14	6*h*	*m*..	0.35897	0.10256	$^1/_4$		coplanar triangle Se_3
Se15	6*h*	*m*..	0.48718	0.28205	$^1/_4$		trigonal bipyramid Cu_5
Cu16	6*h*	*m*..	0.58974	0.02564	$^1/_4$		coplanar triangle Se_3
Cu17	4*f*	3..	$^1/_3$	$^2/_3$	0.107		tetrahedron Se_4
Se18	4*e*	3..	0	0	0.066		tetrahedron $SeCu_3$
Cu19	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		coplanar triangle Se_3
Se20	2*c*	-6..	$^1/_3$	$^2/_3$	$^1/_4$		trigonal bipyramid Cu_5

Transformation from published data: *y*,*x*,-*z*; origin shift 0 0 $^1/_2$

Remarks: Cell parameters and diffraction data (Weissenberg photographs) from [2]. Supersedes a model in space group (194) $P6_3/mmc$ in [3]. In [2] the unit for cell parameters is misprinted as kX instead of Å.

References: [1] Lippmann F. (1962), Neues Jahrb. Mineral., Monatsh. 1962, 99-105. [2] Earley J.W. (1949), Am. Mineral. 34, 435-440. [3] Berry L.G. (1954), Am. Mineral. 39, 504-509.