Cu[SCN]	*hP*8	(186) $P6_3mc$ – b^4

CuNCS β 2H [2]
Structural features: $Cu(S_3N)$ tetrahedra are interconnected via thiocyanate units (linear Cu-N=C=S segments) to form an extended wurtzite-like framework.

Smith D.L., Saunders V.I. (1982) [1]
CCuNS
$a = 0.385$, $c = 1.0937$ nm, $c/a = 2.841$, $V = 0.1404$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
S1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0		single atom C
C2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.1558		single atom N
N3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2564		single atom C
Cu4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4328		tetrahedron NS_3

Transformation from published data ($P6_3mc$ *): *-x,-y,-z*; origin shift $^2/_3$ $^1/_3$ 0.567
Experimental: single crystal, diffractometer, X-rays, R = 0.059, T = 296 K

Remarks: In [1] the origin of the cell is shifted by $^1/_3$ $^2/_3$ 0 from the description in the International Tables for Crystallography.

References: [1] Smith D.L., Saunders V.I. (1982), Acta Crystallogr. B 38, 907-909. [2] Smith D.L., Saunders V.I. (1981), Acta Crystallogr. B 37, 1807-1812.