

$\text{Na}_2\text{Cu}[\text{CN}]_3[\text{H}_2\text{O}]_3$	<i>hP</i> 60	(176) $P6_3/m - i^2h^5ec$
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$\text{Na}_2\text{Cu}(\text{CN})_3 \cdot 3\text{H}_2\text{O}$ [1]

Structural features: Approximately planar $\text{Cu}(\text{CN})_3$ units (perpendicular to [001]; a CuC_3 triangle, linear Cu-C-N segments) in an ordered Mg-type (h.c.p.) arrangement and stacked along the c-axis in a partly disordered arrangement.

Kappenstein C., Hugel R.P. (1978) [1]

$\text{C}_3\text{CuH}_6\text{N}_3\text{Na}_2\text{O}_3$

$a = 1.4582$, $c = 0.3594$ nm, $c/a = 0.246$, $V = 0.6618$ nm³, $Z = 3$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	12 <i>i</i>	1	0.1448	0.0268	0.0831	0.25	non-colinear NC
N2	12 <i>i</i>	1	0.231	0.0429	0.1086	0.25	
Na3	6 <i>h</i>	<i>m</i> ..	0.0201	0.3931	$\frac{1}{4}$		single atom C
N4	6 <i>h</i>	<i>m</i> ..	0.0998	0.6064	$\frac{1}{4}$		
C5	6 <i>h</i>	<i>m</i> ..	0.1864	0.6294	$\frac{1}{4}$		single atom N
(OH ₂)6	6 <i>h</i>	<i>m</i> ..	0.2703	0.0563	$\frac{1}{4}$	0.5	non-colinear Na ₂
(OH ₂)7	6 <i>h</i>	<i>m</i> ..	0.4056	0.2702	$\frac{1}{4}$		
Cu8	4 <i>e</i>	3..	0	0	0.0855	0.25	coplanar triangle C ₃
Cu9	2 <i>c</i>	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		

Experimental: single crystal, diffractometer, X-rays, R = 0.044

Remarks: Average structure; additional reflections could be indexed with a 6-fold supercell (new axes 2a+b, -a+b, 2c). Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kappenstein C., Hugel R.P. (1978), Inorg. Chem. 17, 1945-1949.