

[CN₆H₉]Cl*hP*16(176) *P*6₃/*m* – h²ca**(CH₉N₆)Cl** [2]

Structural features: C(NH-NH₂)₃ units (a central CN₃ triangle; approximately planar except for the terminal H) in a Mg-type (h.c.p.) arrangement.

Bracuti A.J. (1983) [1]

CClH₉N₆*a* = 0.748, *c* = 0.6218 nm, *c/a* = 0.831, *V* = 0.3013 nm³, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
N1	6 <i>h</i>	<i>m</i> ..	0.0204	0.1864	¹ / ₄		non-colinear CN
N2	6 <i>h</i>	<i>m</i> ..	0.3626	0.1591	¹ / ₄		single atom N
Cl3	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		coplanar triangle N ₃
C4	2 <i>a</i>	-6..	0	0	¹ / ₄		coplanar triangle N ₃
H5	12 <i>i</i>	1	0.405	0.144	0.138		
H6	6 <i>h</i>	<i>m</i> ..	0.141	0.291	¹ / ₄		

Transformation from published data: origin shift 0 0 ¹/₂Experimental: single crystal, diffractometer, X-rays, *R* = 0.049

Remarks: 1,2,3-triaminoguanidinium chloride. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bracuti A.J. (1983), *Acta Crystallogr. C* 39, 1465-1467. [2] Okaya Y., Pepinsky R. (1957), *Acta Crystallogr.* 10, 681-684.