NH_4HgCl_3 ($E2_5$) Structure: A3BC_tP5_123_ah_c_b-001

This structure originally had the label `A3BC_tP5_123_cg_a_d`. Calls to that address will be redirected here.

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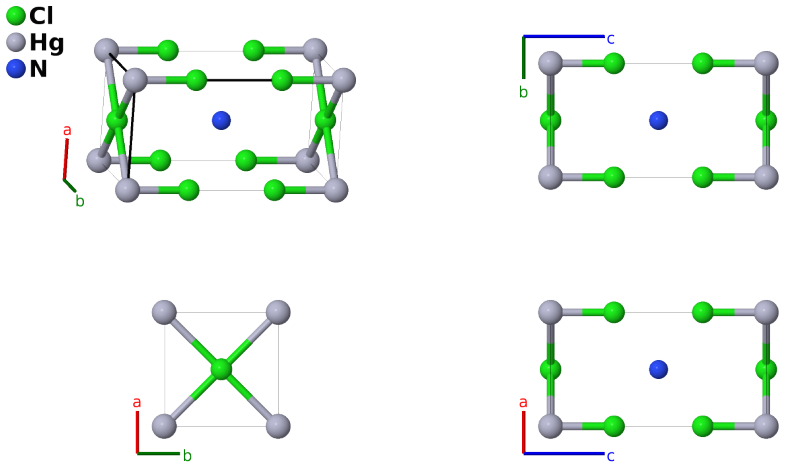
https://aflow.org/p/5MRT

https://aflow.org/p/A3BC_tP5_123_ah_c_b-001

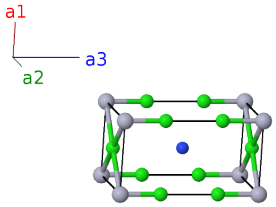


Prototype	$Cl_3H_4HgN_4$
AFLOW prototype label	A3BC_tP5_123_ah_c_b-001
***Strukturbericht* designation**	$E2_5$
ICSD	15962
Pearson symbol	tP5
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A3BC_tP5_123_ah_c_b-001 --params=`$a, c/a, z_4$

- The positions of the hydrogen atoms are not given. It is likely that the hydrogen atoms are freely rotating around the nitrogen, as any reasonable fixed positions would destroy both the inversion symmetry and the four-fold rotation axis exhibited by space group $P4/mmm$ #123.
- (Harmsen, 1939) and (Herrmann, 1943) give multiple possible space groups for this structure. We have chosen the highest symmetry representation, space group $P4/mmm$.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	NH I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(1c)	Hg I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2h)	Cl II
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2h)	Cl II

References

[1] E. J. Harmsen, *The Crystal Structure of NH_4HgCl_3*, Z. Kristallogr. **100**, 208–211 (1939), doi:10.1524/zkri.1939.100.1.208.

Found in

[1] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).