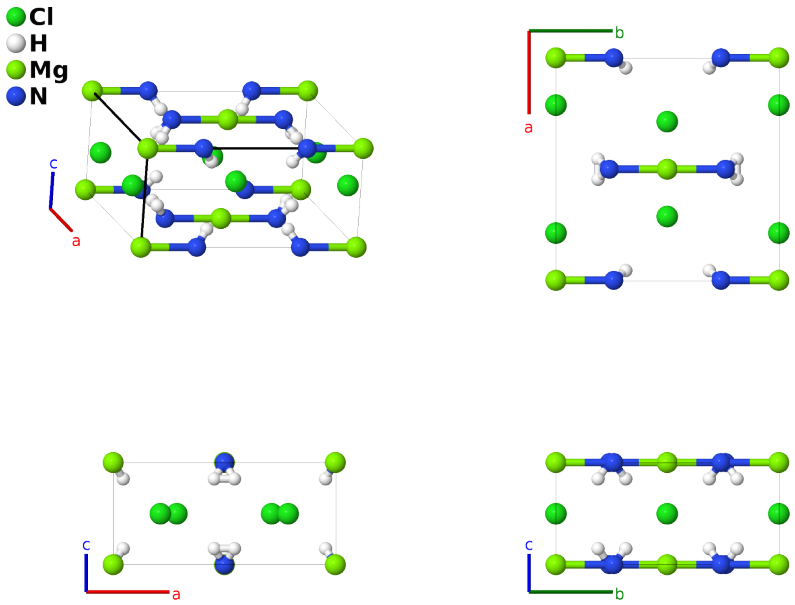
$Mg(NH_3)_2Cl_2$ ($E1_3$) Structure: A2B8CD2_oC26_65_h_r_a_i-001

This structure originally had the label `A2B8CD2_oC26_65_h_r_a_i`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

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

https://aflow.org/p/A2B8CD2_oC26_65_h_r_a_i-001



Prototype	$Cl_2H_6MgN_2$
AFLOW prototype label	A2B8CD2_oC26_65_h_r_a_i-001
***Strukturbericht* designation**	$E1_3$
ICSD	202459
Pearson symbol	oC26
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=A2B8CD2_oC26_65_h_r_a_i-001 --params=`$a, b/a, c/a, x_2, y_3, x_4, y_4, z_4$

Other compounds with this structure

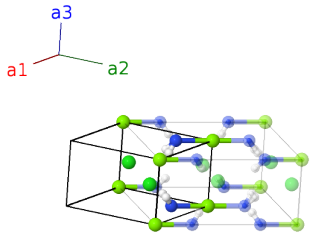
$Cd(NH_3)_2Cl_2$, $Mg(NH_3)_2Cl_2$, $Hg(NH_3)_2Cl_2$, $Ni(NH_3)_2Br_2$, $Ni(NH_3)_2Cl_2$, $Ni(NH_3)_2I_2$

- (Gottfried, 1938) gave the $E1_3$ designation to $Cd(NH_3)_2Cl_2$, and gave coordinates in the $Cmm2$ #35 space group. However, the cited reference, (MacGillavry, 1936) noted that their coordinates allowed several different space groups, with $Cmmm$ #65 having the highest symmetry. We therefore follow most authors and use the $Cmmm$ representation.

- (MacGillavry, 1936) could not determine the positions of the hydrogen atoms, but (Leineweber, 1999) was able to do this using the isostructural compound $Mg(NH_3)_2Cl_2$. Accordingly we us $Mg(NH_3)_2Cl_2$ for the prototype of $E1_3$.
- Twelve hydrogen atoms are statistically distributed among the (16r) positions, giving each site 75% occupation.

Base-centered Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}}\\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Mg I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl I
$\mathbf{B_4}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2$	=	$by_3\,\hat{\mathbf{y}}$	(4i)	N I
$\mathbf{B_5}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2$	=	$-by_3\,\hat{\mathbf{y}}$	(4i)	N I
$\mathbf{B_6}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_7}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_8}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_9}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_{10}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_{11}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_{12}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16r)	H I
$\mathbf{B_{13}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16r)	H I

References

[1] A. Leineweber, M. W. Friedriszik, and H. Jacobs, *Preparation and Crystal Structures of $Mg(NH_3)_2Cl_2$, $Mg(NH_3)_2Br_2$, and $Mg(NH_3)_2I_2$*, J. Solid State Chem. **147**, 229–234 (1999), doi:10.1006/jssc.1999.8238.

[2] C. H. MacGillavry and J. M. Bijvoet, *Die Kristallstruktur von $Zn(NH_3)_2Cl_2$ und $Zn(NH_3)_2Br_2$*, Z. Kristallogr. **94**, 231–245 (1936), doi:10.1524/zkri.1936.94.1.249.

[3] C. Gottfried, ed., *Strukturbericht Band IV 1936* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1938).