

NH₄NO₃ I (*G*0₈) Structure: AB_cP2_221_a_b-001

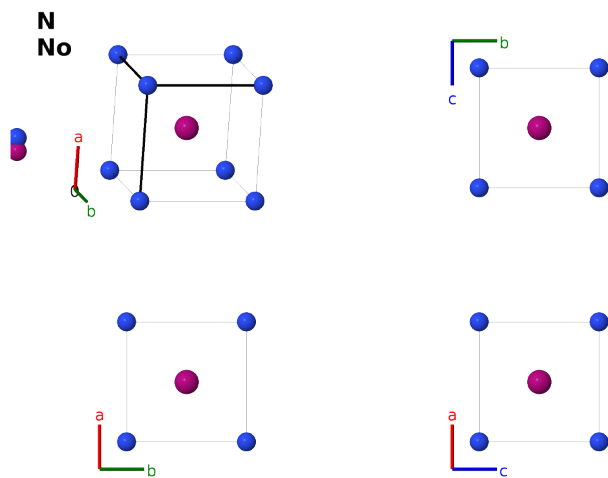
This structure previously used the label(s) **AB_cP2_221_a_b.NH4.NO3**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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/prototype-encyclopedia/5YKM>

https://aflow.org/prototype-encyclopedia/AB_cP2_221_a_b-001



Prototype	(NH ₄)(NO ₃)
AFLOW prototype label	AB_cP2_221_a_b-001
<i>Strukturbericht</i> designation	<i>G</i> 0 ₈
Pearson symbol	cP2
Space group number	221
Space group symbol	<i>Pm</i> $\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_cP2_221_a_b-001 --params=a</code>

- Ammonium Nitrate exists in a variety of forms, (Hermann, 1937) depending on the temperature:

Phase	Temperature °C	<i>Strukturbericht</i>	Page	
I	125 – 170	<i>G</i> 0 ₈	AB_cP2_221_a_b-001	(this structure)
II	84 – 125	<i>G</i> 0 ₉	ABC3_tP10_100_b_a_bc-001	
III	32 – 84	<i>G</i> 0 ₁₀	ABC3_oP20_62_c_c_cd-002	
IV	-18 – 32	<i>G</i> 0 ₁₁	A4B2C3_oP18_59_ef_ab_af-001	
V	< -18		A4B2C3_tP72_77_8d_ab2c2d_6d2-001	

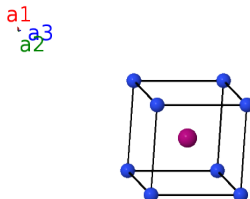
- In the $G0_8$ structure, both the NH_4 and NO_3 radicals rotate freely about their centers of mass (Kracek, 1931). The two radicals sit on the same sites as atoms in the CsCl ($B2$) structure.

Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = a \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(1a) NH I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(1b) NO I

References

- [1] F. C. Kracek, S. B. Hendricks, and E. Posnjak, *Group Rotation in Solid Ammonium and Calcium Nitrates*, Nature **128**, 410–411 (1931), doi:10.1038/128410b0.
- [2] S. B. Hendricks, E. Posnjak, and F. C. Kracek, *Molecular Rotation in the Solid State. The Variation of the Crystal Structure of Ammonium Nitrate with Temperature*, J. Am. Chem. Soc. **54**, 2766–2786 (1932), doi:10.1021/ja01346a020.

Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

First cited in

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.