NH_4NO_3 I ($G0_8$) Structure: AB_cP2_221_a_b-001

This structure originally had the label `AB_cP2_221_a_b.NH4.NO3`. Calls to that address will be redirected here.

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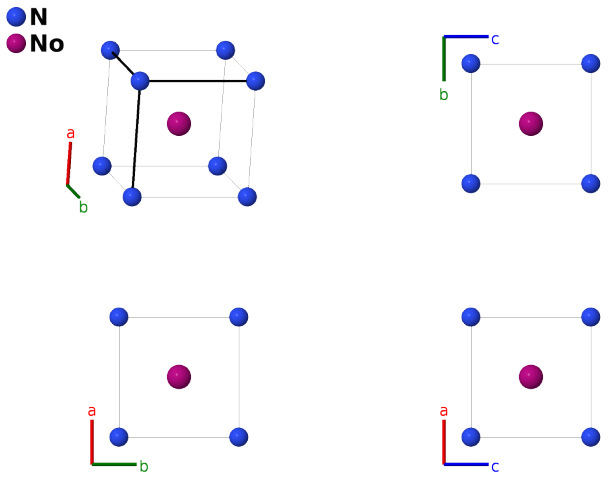
https://aflow.org/p/5YKM

https://aflow.org/p/AB_cP2_221_a_b-001



Prototype	$(NH_4)(NO_3)$
AFLOW prototype label	AB_cP2_221_a_b-001
***Strukturbericht* designation**	$G0_8$
ICSD	none
Pearson symbol	cP2
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cP2_221_a_b-001 --params=`a

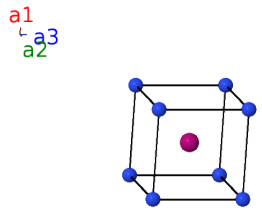
- Ammonium Nitrate exists in a variety of forms, (Hermann, 1937) depending on the temperature:

Phase	Temperature °C	*Strukturbericht*	Page	
I	125 – 170	$G0_8$	AB_cP2_221_a_b-001	(this structure)
II	84 – 125	$G0_9$	ABC3_tP10_100_b_a_bc	
III	32 – 84	$G0_{10}$	ABC3_oP20_62_c_c_cd-002	
IV	-18 – 32	$G0_{11}$	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 Soid 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).