NH_4NO_3 II ($G0_9$) Structure: ABC3_tP10_100_b_a_bc-001

This structure originally had the label `ABC3_tP10_100_b_a_bc`. Calls to that address will be redirected here.

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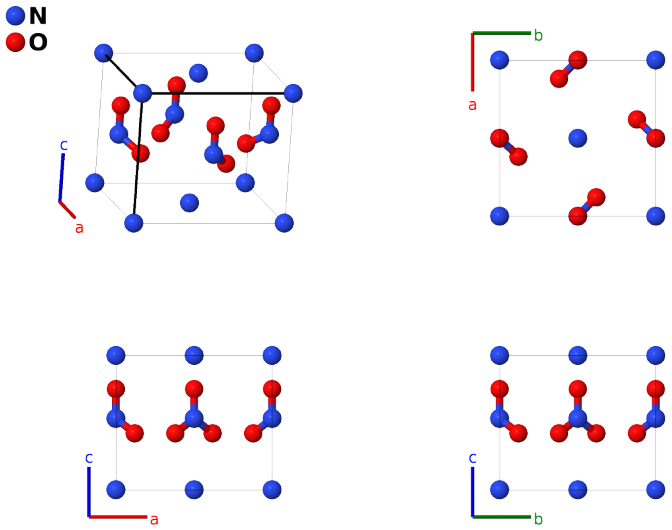
https://aflow.org/p/80PK

https://aflow.org/p/ABC3_tP10_100_b_a_bc-001



Prototype	$N(NH_4)O_3$
AFLOW prototype label	ABC3_tP10_100_b_a_bc-001
***Strukturbericht* designation**	$G0_9$
ICSD	none
Pearson symbol	tP10
Space group number	100
Space group symbol	*P4bm*
AFLOW prototype command	`aflow --proto=ABC3_tP10_100_b_a_bc-001 --params=`$a, c/a, z_1, z_2, z_3, x_4, z_4$

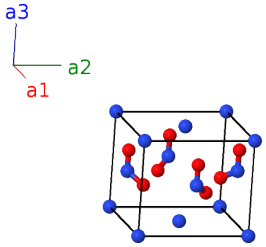
- Ammonium Nitrate exists in a variety of forms, (Hermann, 1937) depending on the temperature:

Phase	Temperature °C	*Strukturbericht*	Page	
I	125 – 170	$G0_8$	AB_cP2_221_a_b-001	
II	84 – 125	$G0_9$	ABC3_tP10_100_b_a_bc	(this structure)
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	

- Data for this structure was taken at 60°C.
- The positions of the hydrogen atoms were not determined. The isolated nitrogen atoms in this structure's visualization are surrounded by four hydrogen atoms in an approximately tetrahedral arrangement. It is likely that the NH_4 radicals are free to rotate (Kracek, 1937).
- Both (Shinnaka, 1956) and (Hermann, 1937) state that the available X-ray diffraction data supports a space group of either $P4bm$ #100 or $P\bar{4}2_1m$ #113. The atomic positions found by Shinnaka agree with space group $P4bm$.
- (Shinnaka, 1956) states that the NO_3 nitrate groups are rotating, but this rotation "is almost bound in two orientations (in opposite directions)." He then gives two possible orientations for the nitrate. We present the first orientation here. The second orientation is obtained by taking $z_3 \to -z_3$ and $z_4 \to -z_4$.
- Another way of presenting this information would be to add a second nitrate group to the primitive cell, and set the occupation of all the atoms in the nitrates at 50%. This would give a structure in space group $P4/mbm$ #127, which might be useful as a pictorial representation but does not correctly represent the physics of the crystal, as the nitrogen and oxygen atoms in an individual nitrate radical must remain together.
- The N–O distances in this structure are about 10% smaller than the distances found in the other phases of NH_4NO_3. This suggests that the structure should be reevaluated.

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
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	NH I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(2a)	NH I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_2\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2b)	N I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_9}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II
$\mathbf{B_{10}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4c)	O II

References

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