$AgNO_2$ ($F5_{12}$) Structure: ABC2_oI8_44_a_a_c-002

This structure originally had the label `ABC2_oI8_44_a_a_d`. Calls to that address will be redirected here.

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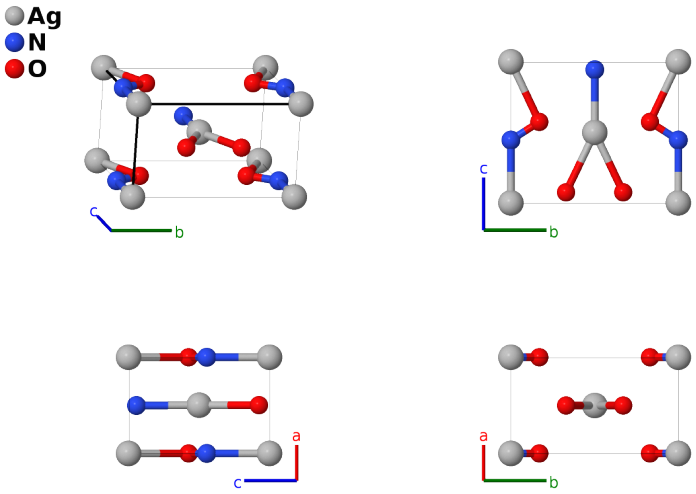
https://aflow.org/p/VTNW

https://aflow.org/p/ABC2_oI8_44_a_a_c-002



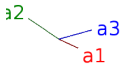
Prototype	$AgNO_2$
AFLOW prototype label	ABC2_oI8_44_a_a_c-002
***Strukturbericht* designation**	$F5_{12}$
Mineral name	silver nitrite
ICSD	24378
Pearson symbol	oI8
Space group number	44
Space group symbol	$Imm2$
AFLOW prototype command	`aflow --proto=ABC2_oI8_44_a_a_c-002 --params=`$a, b/a, c/a, z_1, z_2, x_3, z_3$

Other compounds with this structure
$NaNO_3$ ($F5_5$)

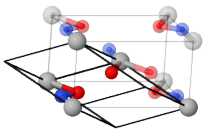
- This structure is very similar to sodium nitrite, $NbNO_2$, $F5_5$.
- We list both structures as they have separate entries in the *Strukturbericht* volumes.

- The original publications give Wyckoff positions giving $NaNO_2$ the AFLOW prototype label ABC2_oI8_44_a_a_c and $AgNO_2$ the label ABC2_oI8_44_a_a_d. When we apply our AFLOW prototype label rules, however, the label for both structures becomes ABC2_oI8_44_a_a_c. The two structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- The origin of the z coordinate in $Imm2$ #44 is arbitrary, and we set z_1 to zero.

Body-centered Orthorhombic primitive vectors



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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_1 + z_1\,\mathbf{a}_2$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Ag I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	N I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_1 + (x_3 + z_3)\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 - (x_3 - z_3)\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I

References

[1] S. Ohba and Y. Saito, *Structure of silver(I) nitrite, a redetermination*, Acta Crystallogr. Sect. B **37**, 1911–1913 (1981), doi:10.1107/S0567740881007565.