$CsHgN_3O_6$ Structure: ABC3D6_cP11_200_a_b_c_f-001

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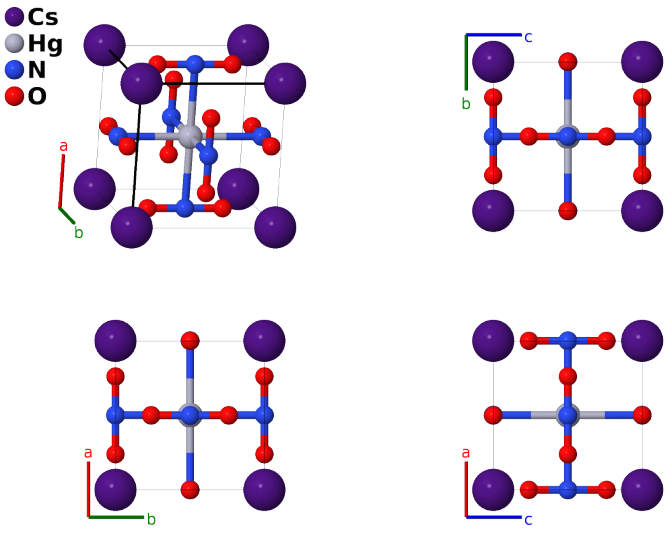
https://aflow.org/p/4JP4

https://aflow.org/p/ABC3D6_cP11_200_a_b_c_f-001



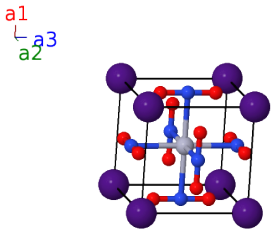
Prototype	$CsHgN_3O_6$
AFLOW prototype label	ABC3D6_cP11_200_a_b_c_f-001
ICSD	28645
Pearson symbol	cP11
Space group number	200
Space group symbol	$Pm\overline{3}$
AFLOW prototype command	`aflow --proto=ABC3D6_cP11_200_a_b_c_f-001 --params=`a, x_4

Other compounds with this structure

$CsCdN_3O_6$, $KHgN_3O_6$, $RbCdN_3O_6$, $RbHgN_3O_6$, $TlCdN_3O_6$, $TlHgN_3O_6$

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)	Cs 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)	Hg I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	N I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	N I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	N I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(6f)	O I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + ax_4\,\hat{\mathbf{z}}$	(6f)	O I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} - ax_4\,\hat{\mathbf{z}}$	(6f)	O I

References

[1] A. Ferrari and C. Colla, *Mercurinitriti di metalli monovalenti*, Gazz. Chim. Ital. **65**, 789–797 (1935).

Found in

[1] *Crystallography Open Database*. Information card for entry 1010350.