Na_2HgO_2 Structure: AB2C2_tI10_139_a_e_e-001

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https://aflow.org/p/6LGV

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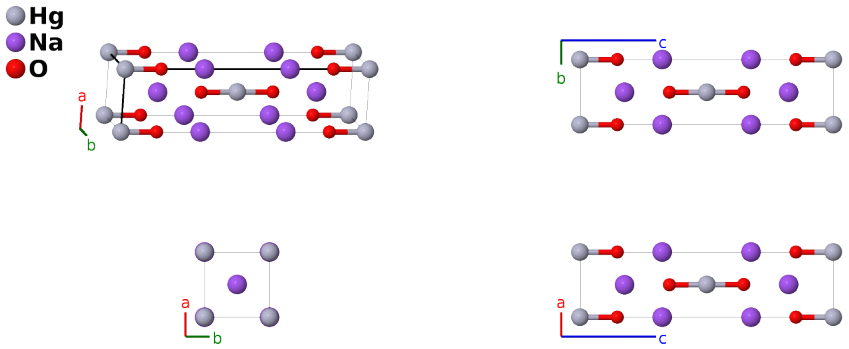


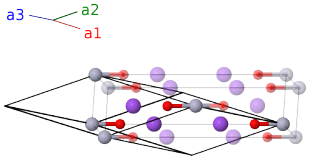
Prototype	$HgNa_2O_2$
AFLOW prototype label	AB2C2_tI10_139_a_e_e-001
ICSD	25511
Pearson symbol	tI10
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2C2_tI10_139_a_e_e-001 --params=`$a, c/a, z_2, z_3$

Other compounds with this structure
Cs_2HgO_2, Li_2HgO_2, Rb_2HgO_2, U_2IrC_2, U_2RuC_2

- (Hoppe, 1964) give the space group as $I422$ #97, but the Wyckoff positions they use are consistent with $I4/mmm$ #139, so we use the higher symmetry space group.

Body-centered Tetragonal primitive vectors

$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - \frac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Hg I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_3}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_4}$	=	$z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$	=	$cz_3\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_5}$	=	$-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	O I

References

[1] R. Hoppe and H.-J. Rohrborn, *Oxomercurate(II) der Alkalimetalle, M_2HgO_2*, Zeitschrift für anorganische und allgemeine Chemie **329**, 110–122 (1964), doi:10.1002/zaac.19643290115.