

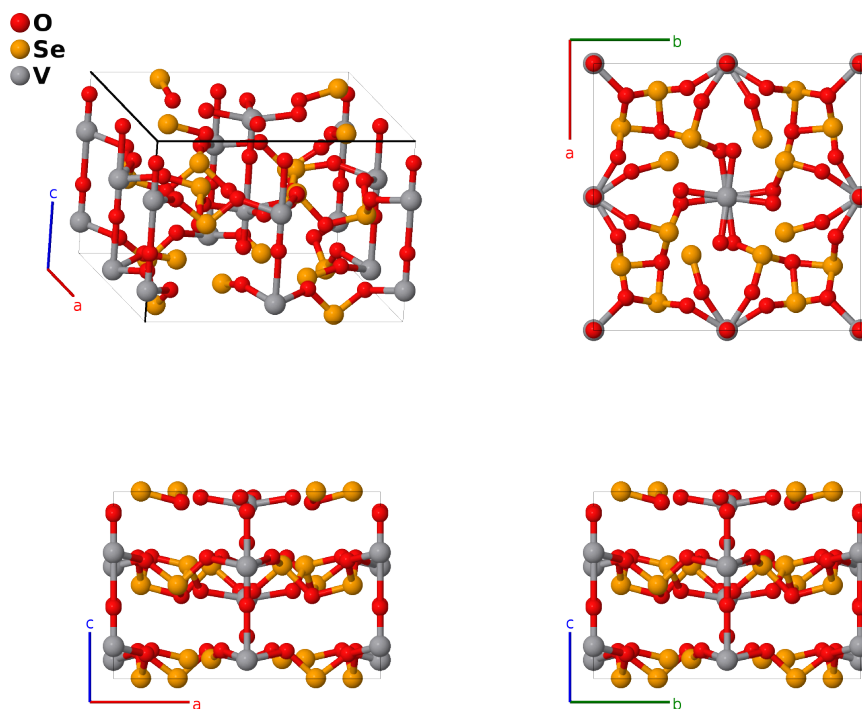
# VSe<sub>2</sub>O<sub>6</sub> Structure: A6B2C\_tP72\_103\_abc5d\_2d\_abc-001

This structure originally had the label A6B2C\_tP72\_103\_abc5d\_2d\_abc. Calls to that address will be redirected here.

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<https://afLOW.org/p/9ZX1>

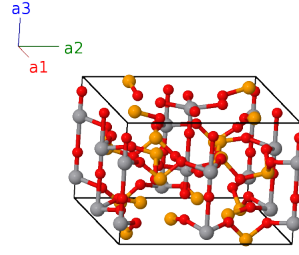
[https://afLOW.org/p/A6B2C\\_tP72\\_103\\_abc5d\\_2d\\_abc-001](https://afLOW.org/p/A6B2C_tP72_103_abc5d_2d_abc-001)



Prototype	O <sub>6</sub> Se <sub>2</sub> V
AFLOW prototype label	A6B2C_tP72_103_abc5d_2d_abc-001
ICSD	2354
Pearson symbol	tP72
Space group number	103
Space group symbol	<i>P4cc</i>
AFLOW prototype command	afLOW --proto=A6B2C_tP72_103_abc5d_2d_abc-001 --params= <i>a, c/a, z<sub>1</sub>, z<sub>2</sub>, z<sub>3</sub>, z<sub>4</sub>, z<sub>5</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub>, x<sub>11</sub>, y<sub>11</sub>, z<sub>11</sub>, x<sub>12</sub>, y<sub>12</sub>, z<sub>12</sub>, x<sub>13</sub>, y<sub>13</sub>, z<sub>13</sub></i>

Simple Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$




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## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= z_1 \mathbf{a}_3$	$=$	$c z_1 \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_2$	$= (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$c z_2 \hat{\mathbf{z}}$	(2a)	V I
$\mathbf{B}_4$	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c (z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(2a)	V I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	O II
$\mathbf{B}_7$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c z_4 \hat{\mathbf{z}}$	(2b)	V II
$\mathbf{B}_8$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}} + c (z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(2b)	V II
$\mathbf{B}_9$	$= \frac{1}{2} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_5 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{10}$	$= \frac{1}{2} \mathbf{a}_1 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_5 \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{11}$	$= \frac{1}{2} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{12}$	$= \frac{1}{2} \mathbf{a}_1 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c (z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	O III
$\mathbf{B}_{13}$	$= \frac{1}{2} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c z_6 \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{14}$	$= \frac{1}{2} \mathbf{a}_1 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c z_6 \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{15}$	$= \frac{1}{2} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{16}$	$= \frac{1}{2} \mathbf{a}_1 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + c (z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	V III
$\mathbf{B}_{17}$	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} + a y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{18}$	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} - a y_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{19}$	$= -y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$-a y_7 \hat{\mathbf{x}} + a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{20}$	$= y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$a y_7 \hat{\mathbf{x}} - a x_7 \hat{\mathbf{y}} + c z_7 \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{21}$	$= x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_7 \hat{\mathbf{x}} - a y_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{22}$	$= -x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_7 \hat{\mathbf{x}} + a y_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{23}$	$= -y_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a y_7 \hat{\mathbf{x}} - a x_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{24}$	$= y_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a y_7 \hat{\mathbf{x}} + a x_7 \hat{\mathbf{y}} + c (z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O IV
$\mathbf{B}_{25}$	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a x_8 \hat{\mathbf{x}} + a y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{26}$	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a x_8 \hat{\mathbf{x}} - a y_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{27}$	$= -y_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$-a y_8 \hat{\mathbf{x}} + a x_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{28}$	$= y_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$a y_8 \hat{\mathbf{x}} - a x_8 \hat{\mathbf{y}} + c z_8 \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{29}$	$= x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a x_8 \hat{\mathbf{x}} - a y_8 \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V
$\mathbf{B}_{30}$	$= -x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a x_8 \hat{\mathbf{x}} + a y_8 \hat{\mathbf{y}} + c (z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(8d)	O V



$$\mathbf{B}_{72} = y_{13} \mathbf{a}_1 + x_{13} \mathbf{a}_2 + \left(z_{13} + \frac{1}{2}\right) \mathbf{a}_3 = ay_{13} \hat{\mathbf{x}} + ax_{13} \hat{\mathbf{y}} + c \left(z_{13} + \frac{1}{2}\right) \hat{\mathbf{z}} \quad (8d) \quad \text{Se II}$$

## References

- [1] G. Meunier, M. Bertaud, and J. Galy, *Cristallochimie du sélénium(+IV). I.  $VSe_2O_6$ , une structure à trois chaînes parallèles  $(VO_5)_n^{6n-}$  indépendantes pontées par des groupements  $(Se_2O)^{6+}$* , Acta Crystallogr. Sect. B **30**, 2834–2839 (1974), doi:10.1107/S0567740874008260.