

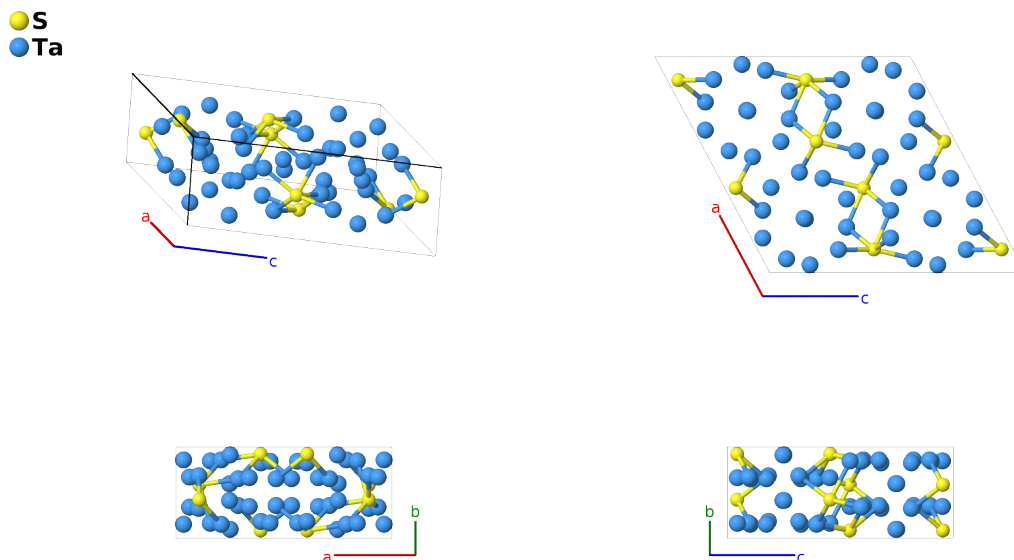
Ta₆S Structure:

AB6_mC56_15_f_6f-001

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<https://afLOW.org/p/HXME>

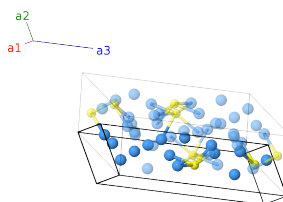
https://afLOW.org/p/AB6_mC56_15_f_6f-001



Prototype	STa ₆
AFLOW prototype label	AB6_mC56_15_f_6f-001
ICSD	16041
Pearson symbol	mC56
Space group number	15
Space group symbol	<i>C</i> 2/ <i>c</i>
AFLOW prototype command	afLOW --proto=AB6_mC56_15_f_6f-001 --params= <i>a</i> , <i>b/a</i> , <i>c/a</i> , β , <i>x</i> ₁ , <i>y</i> ₁ , <i>z</i> ₁ , <i>x</i> ₂ , <i>y</i> ₂ , <i>z</i> ₂ , <i>x</i> ₃ , <i>y</i> ₃ , <i>z</i> ₃ , <i>x</i> ₄ , <i>y</i> ₄ , <i>z</i> ₄ , <i>x</i> ₅ , <i>y</i> ₅ , <i>z</i> ₅ , <i>x</i> ₆ , <i>y</i> ₆ , <i>z</i> ₆ , <i>x</i> ₇ , <i>y</i> ₇ , <i>z</i> ₇

Base-centered Monoclinic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= (x_1 - y_1) \mathbf{a}_1 + (x_1 + y_1) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$= (ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_2	$= -(x_1 + y_1) \mathbf{a}_1 - (x_1 - y_1) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_3	$= -(x_1 - y_1) \mathbf{a}_1 - (x_1 + y_1) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$= -(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_4	$= (x_1 + y_1) \mathbf{a}_1 + (x_1 - y_1) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$= (ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	S I
\mathbf{B}_5	$= (x_2 - y_2) \mathbf{a}_1 + (x_2 + y_2) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$= (ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_6	$= -(x_2 + y_2) \mathbf{a}_1 - (x_2 - y_2) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_7	$= -(x_2 - y_2) \mathbf{a}_1 - (x_2 + y_2) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$= -(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_8	$= (x_2 + y_2) \mathbf{a}_1 + (x_2 - y_2) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$= (ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta I
\mathbf{B}_9	$= (x_3 - y_3) \mathbf{a}_1 + (x_3 + y_3) \mathbf{a}_2 + z_3 \mathbf{a}_3$	$= (ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta II
\mathbf{B}_{10}	$= -(x_3 + y_3) \mathbf{a}_1 - (x_3 - y_3) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta II
\mathbf{B}_{11}	$= -(x_3 - y_3) \mathbf{a}_1 - (x_3 + y_3) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$= -(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta II
\mathbf{B}_{12}	$= (x_3 + y_3) \mathbf{a}_1 + (x_3 - y_3) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$= (ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta II
\mathbf{B}_{13}	$= (x_4 - y_4) \mathbf{a}_1 + (x_4 + y_4) \mathbf{a}_2 + z_4 \mathbf{a}_3$	$= (ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta III
\mathbf{B}_{14}	$= -(x_4 + y_4) \mathbf{a}_1 - (x_4 - y_4) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta III
\mathbf{B}_{15}	$= -(x_4 - y_4) \mathbf{a}_1 - (x_4 + y_4) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$= -(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta III
\mathbf{B}_{16}	$= (x_4 + y_4) \mathbf{a}_1 + (x_4 - y_4) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$= (ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta III
\mathbf{B}_{17}	$= (x_5 - y_5) \mathbf{a}_1 + (x_5 + y_5) \mathbf{a}_2 + z_5 \mathbf{a}_3$	$= (ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta IV
\mathbf{B}_{18}	$= -(x_5 + y_5) \mathbf{a}_1 - (x_5 - y_5) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta IV
\mathbf{B}_{19}	$= -(x_5 - y_5) \mathbf{a}_1 - (x_5 + y_5) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$= -(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta IV
\mathbf{B}_{20}	$= (x_5 + y_5) \mathbf{a}_1 + (x_5 - y_5) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$= (ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta IV
\mathbf{B}_{21}	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$= (ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8f)	Ta V
\mathbf{B}_{22}	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$= -(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(8f)	Ta V

$$\mathbf{B}_{23} = \begin{matrix} -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - \\ z_6 \mathbf{a}_3 \end{matrix} = -(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Ta V}$$

$$\mathbf{B}_{24} = \begin{matrix} (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + \\ (z_6 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_6 + c(z_6 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + \\ c(z_6 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta V}$$

$$\mathbf{B}_{25} = \begin{matrix} (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + \\ z_7 \mathbf{a}_3 \end{matrix} = (ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Ta VI}$$

$$\mathbf{B}_{26} = \begin{matrix} -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - \\ (z_7 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} -(ax_7 + c(z_7 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - \\ c(z_7 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta VI}$$

$$\mathbf{B}_{27} = \begin{matrix} -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - \\ z_7 \mathbf{a}_3 \end{matrix} = -(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}} \quad (8f) \quad \text{Ta VI}$$

$$\mathbf{B}_{28} = \begin{matrix} (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + \\ (z_7 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = \begin{matrix} (ax_7 + c(z_7 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + \\ c(z_7 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \end{matrix} \quad (8f) \quad \text{Ta VI}$$

References

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