

Rh₃S₄:

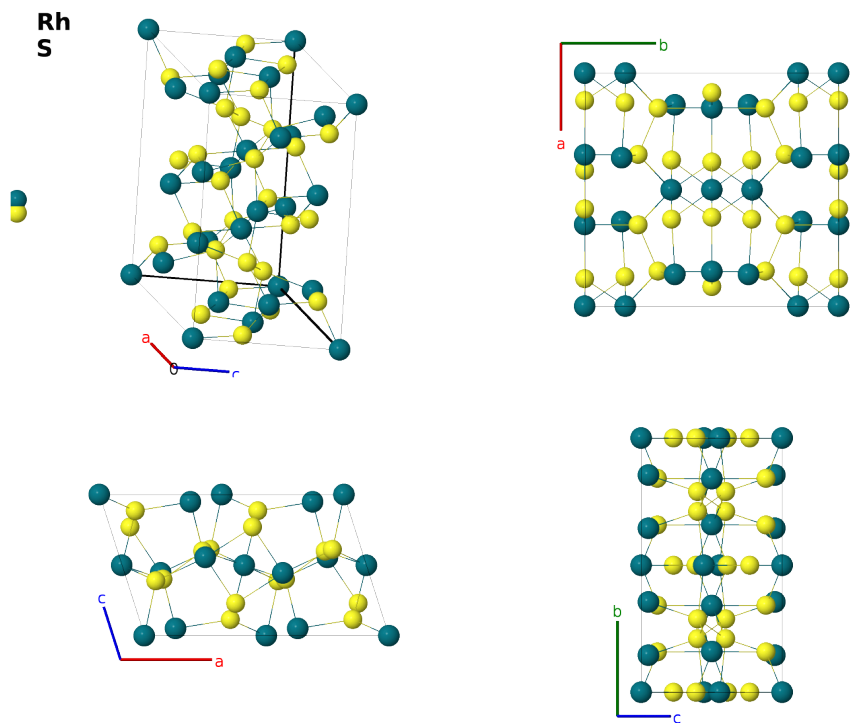
A3B4_mC42_12_ahij_2i2j-001

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<https://aflow.org/prototype-encyclopedia/F2JA>

https://aflow.org/prototype-encyclopedia/A3B4_mC42_12_ahij_2i2j-001



Prototype	Rh ₃ S ₄
AFLOW prototype label	A3B4_mC42_12_ahij_2i2j-001
ICSD	410813
CCDC	1726572
Pearson symbol	mC42
Space group number	12
Space group symbol	C2/m
AFLOW prototype command	<code>aflow --proto=A3B4_mC42_12_ahij_2i2j-001</code> <code>--params=a,b/a,c/a,β,y₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈,z₈</code>

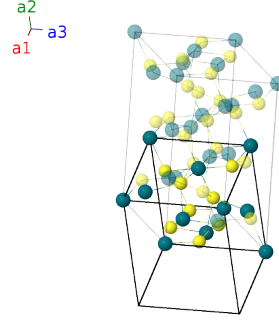
Other compounds with this structure

Rh₃Se₄

- This is a laboratory produced sample. The minerals kingstonite, $(\text{Rh},\text{Ir})_3\text{S}_4$, and zaykovite, $(\text{Rh},\text{Pt},\text{Ir})_3(\text{Se},\text{S})_4$, are naturally occurring compounds with this structure. (Belogub, 2023)

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
$\mathbf{B}_1$	$= 0$	$=$	0	(2a)	Rh I
$\mathbf{B}_2$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Rh II
$\mathbf{B}_3$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Rh II
$\mathbf{B}_4$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Rh III
$\mathbf{B}_5$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	Rh III
$\mathbf{B}_6$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B}_7$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	S I
$\mathbf{B}_8$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B}_9$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	S II
$\mathbf{B}_{10}$	$= (x_6 - y_6) \mathbf{a}_1 + (x_6 + y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Rh IV
$\mathbf{B}_{11}$	$= -(x_6 + y_6) \mathbf{a}_1 - (x_6 - y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Rh IV
$\mathbf{B}_{12}$	$= -(x_6 - y_6) \mathbf{a}_1 - (x_6 + y_6) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Rh IV
$\mathbf{B}_{13}$	$= (x_6 + y_6) \mathbf{a}_1 + (x_6 - y_6) \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(8j)	Rh IV
$\mathbf{B}_{14}$	$= (x_7 - y_7) \mathbf{a}_1 + (x_7 + y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	S III
$\mathbf{B}_{15}$	$= -(x_7 + y_7) \mathbf{a}_1 - (x_7 - y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	S III
$\mathbf{B}_{16}$	$= -(x_7 - y_7) \mathbf{a}_1 - (x_7 + y_7) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	S III
$\mathbf{B}_{17}$	$= (x_7 + y_7) \mathbf{a}_1 + (x_7 - y_7) \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(8j)	S III
$\mathbf{B}_{18}$	$= (x_8 - y_8) \mathbf{a}_1 + (x_8 + y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	S IV
$\mathbf{B}_{19}$	$= -(x_8 + y_8) \mathbf{a}_1 - (x_8 - y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(8j)	S IV

$$\mathbf{B}_{20} = - (x_8 - y_8) \mathbf{a}_1 - (x_8 + y_8) \mathbf{a}_2 - z_8 \mathbf{a}_3 = - (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}} \quad (8j) \quad \text{S IV}$$

$$\mathbf{B}_{21} = (x_8 + y_8) \mathbf{a}_1 + (x_8 - y_8) \mathbf{a}_2 + z_8 \mathbf{a}_3 = (ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}} \quad (8j) \quad \text{S IV}$$

References

- [1] J. Beck and T. Hilbert, *An ‘old’ Rhodiumsulfide with surprising Structure – Synthesis, Crystal Structure, and Electronic Properties of Rh_3S_4* , Z. Anorganische und Allgemeine Chemie **626**, 729–9 (2000), doi:10.1002/(SICI)1521-3749(200001)626:1<72::AID-ZAAC72>3.0.CO;2-I.

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- [1] E. V. Belogub, S. N. Britvin, V. V. Shilovskikh, L. A. Pautov, V. A. Kotlyarov, and E. V. Zaykova, *Zaykovite, Rh_3Se_4 , a new mineral from the Kazan placer, South Urals, Russia*, Mineral. Mag. **87**, 118–129 (2023), doi:10.1180/mgm.2022.122.

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