

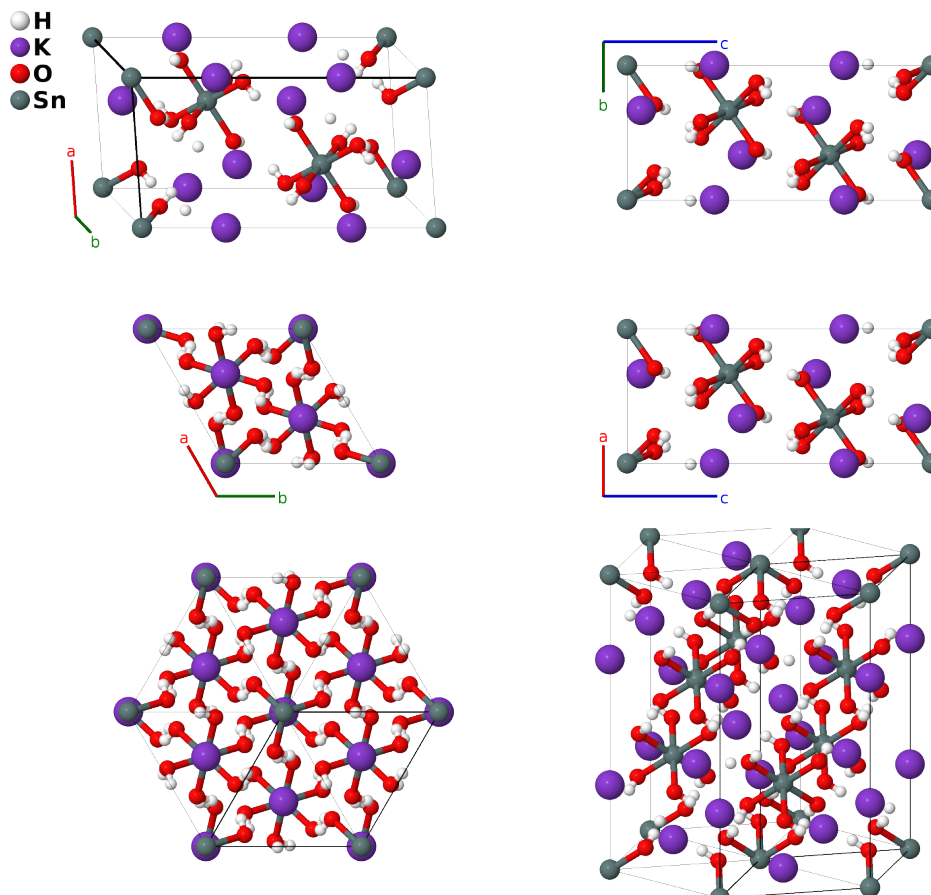
# $K_2Sn(OH)_6$ ( $H6_2$ ) Structure: A6B2C6D\_hR15\_148\_f\_c\_f\_a-001

This structure originally had the label A6B2C6D\_hR15\_148\_f\_c\_f\_a. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/p/FKGA>

[https://aflow.org/p/A6B2C6D\\_hR15\\_148\\_f\\_c\\_f\\_a-001](https://aflow.org/p/A6B2C6D_hR15_148_f_c_f_a-001)



Prototype	$H_6K_2O_6Sn$
AFLOW prototype label	A6B2C6D_hR15_148_f_c_f_a-001
<i>Strukturbericht</i> designation	$H6_2$
ICSD	92465
Pearson symbol	hR15
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	<code>aflow --proto=A6B2C6D_hR15_148_f_c_f_a-001 --params=a, c/a, x2, x3, y3, z3, x4, y4, z4</code>

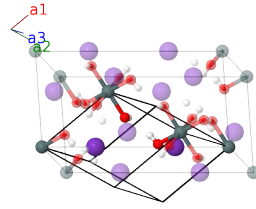
## Other compounds with this structure

$\text{K}_2\text{Pt}(\text{OH})_6$ ,  $\text{Na}_2\text{Sn}(\text{OH})_6$

- (Wyckoff, 1928) found the positions of the potassium and tin atoms in this structure. He could not locate the oxygen atoms, and so was unable to give an unequivocal determination of the space group, beyond noting that it was rhombohedral. We use the modern structure of (Jacobs, 2000), which agrees with Wyckoff in the positioning of the potassium and tin atoms and finds both the hydrogen and oxygen locations.
- (Ewald, 1931) gave this the *Strukturbericht* designation  $H6_2$ . (Hermann, 1937) began relabeling the  $H6$  structures as  $I1$ , and (Gottfried, 1937) relabeled them as  $J1$ , but neither they nor successor volumes revisited this structure, so it was never formally relabeled  $J1_2$ . We will therefore leave it as  $H6_2$ .
- Hexagonal settings for rhombohedral structures can be obtained with the option `--hex`.

## Rhombohedral primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{\sqrt{3}}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= -\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{3}c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	$0$	$=$	$0$	(1a) Sn I
$\mathbf{B}_2$	$=$	$x_2 \mathbf{a}_1 + x_2 \mathbf{a}_2 + x_2 \mathbf{a}_3$	$=$	$cx_2 \hat{\mathbf{z}}$	(2c) K I
$\mathbf{B}_3$	$=$	$-x_2 \mathbf{a}_1 - x_2 \mathbf{a}_2 - x_2 \mathbf{a}_3$	$=$	$-cx_2 \hat{\mathbf{z}}$	(2c) K I
$\mathbf{B}_4$	$=$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_5$	$=$	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_7$	$=$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_8$	$=$	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_9$	$=$	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) H I
$\mathbf{B}_{10}$	$=$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f) O I
$\mathbf{B}_{11}$	$=$	$z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f) O I
$\mathbf{B}_{12}$	$=$	$y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f) O I
$\mathbf{B}_{13}$	$=$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f) O I

$$\mathbf{B}_{14} = -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 = \frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} \quad (6f) \quad \text{O I}$$

$$\mathbf{B}_{15} = -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 = \frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} \quad (6f) \quad \text{O I}$$

## References

- [1] H. Jacobs and R. Stahl, *Neubestimmung der Kristallstrukturen der Hexahydroxometallate  $\text{Na}_2\text{Sn}(\text{OH})_6$ ,  $\text{K}_2\text{Sn}(\text{OH})_6$  und  $\text{K}_2\text{Pb}(\text{OH})_6$* , Z. Anorganische und Allgemeine Chemie **626**, 1863–1866 (2000), doi:10.1002/1521-3749(200009)626:9<1863::AID-ZAAC1863>3.0.CO;2-M.
- [2] R. W. G. Wyckoff, *The Crystal Structure of Potassium Hydroxystannate,  $\text{K}_2\text{Sn}(\text{OH})_6$* , Am. J. Sci. **15**, 297–302 (1928), doi:10.2475/ajs.s5-15.88.297.
- [3] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [4] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [5] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

## Found in

- [1] P. Villars,  *$\text{K}_2\text{Sn}(\text{OH})_6$  ( $\text{K}_2\text{Sn}[\text{OH}]_6$ ) Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) Springer Materials.