

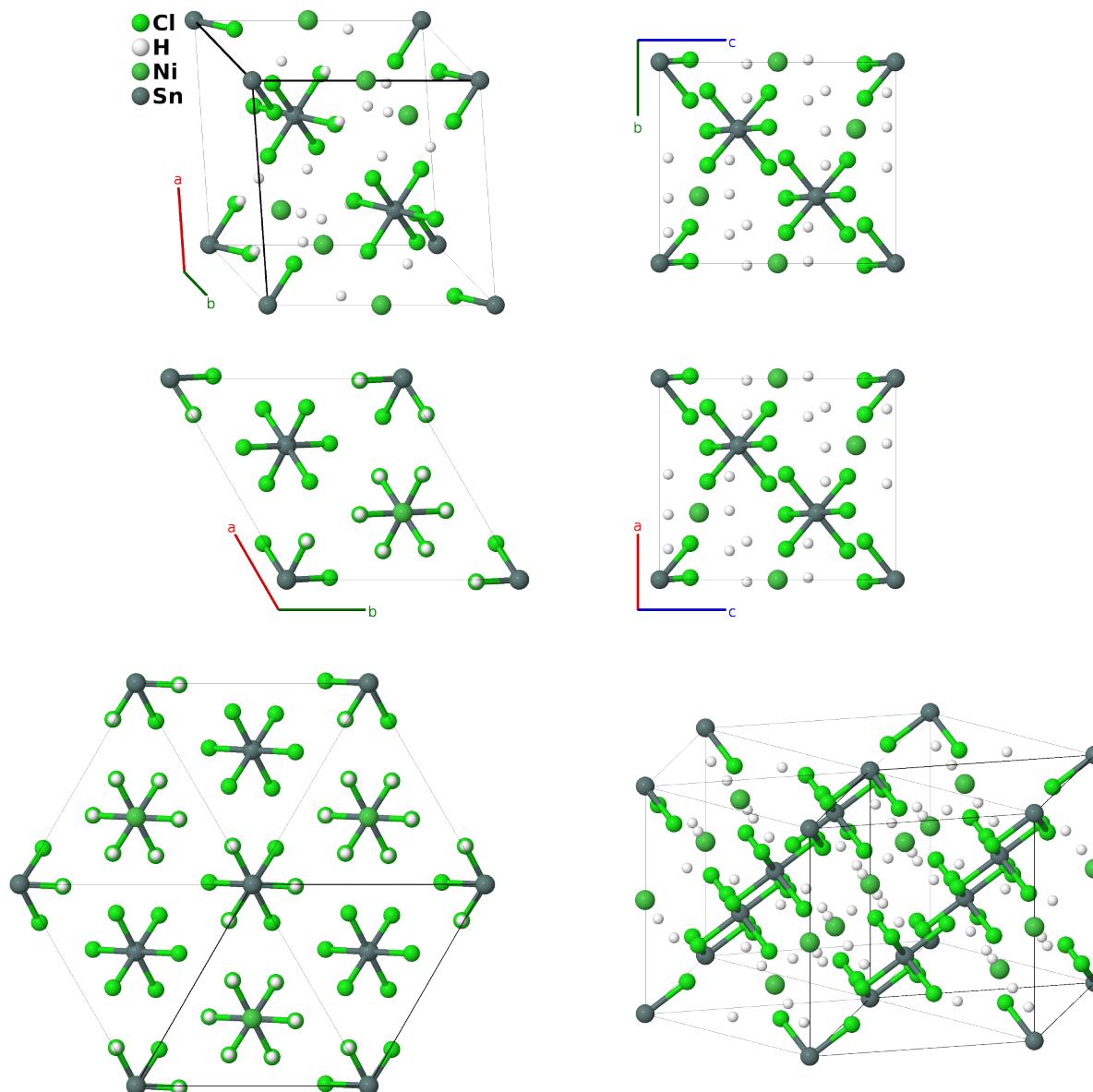
# Ni(H<sub>2</sub>O)<sub>6</sub>SnCl<sub>6</sub> (*I*6<sub>1</sub>) Structure: A6B6CD\_hR14\_148\_f\_f\_a\_b-001

This structure originally had the label A6B6CD\_hR14\_148\_f\_f\_b.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/5954>

[https://aflow.org/p/A6B6CD\\_hR14\\_148\\_f\\_f\\_a\\_b-001](https://aflow.org/p/A6B6CD_hR14_148_f_f_a_b-001)



Prototype	Cl <sub>6</sub> (H <sub>2</sub> O) <sub>6</sub> NiSn
AFLOW prototype label	A6B6CD_hR14_148_f_f_a_b-001
<i>Strukturbericht</i> designation	<i>I</i> 6 <sub>1</sub>

ICSD	26679
Pearson symbol	hR14
Space group number	148
Space group symbol	$R\bar{3}$
AFLOW prototype command	aflow --proto=A6B6CD_hR14_148_f_f_a_b-001 --params=a, c/a, x <sub>3</sub> , y <sub>3</sub> , z <sub>3</sub> , x <sub>4</sub> , y <sub>4</sub> , z <sub>4</sub>

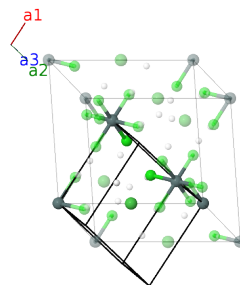
### Other compounds with this structure

Ca(H<sub>2</sub>O)<sub>6</sub>SnF<sub>6</sub>, Co(H<sub>2</sub>O)<sub>6</sub>PtF<sub>6</sub>, Co(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Co(NH<sub>3</sub>)<sub>6</sub>Co(CN)<sub>6</sub>, Fe(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Mg(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Mg(H<sub>2</sub>O)<sub>6</sub>SnF<sub>6</sub>, Mg(H<sub>2</sub>O)<sub>6</sub>TiF<sub>6</sub>, Mn(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Ni(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Zn(H<sub>2</sub>O)<sub>6</sub>SiF<sub>6</sub>, Zn(H<sub>2</sub>O)<sub>6</sub>SnF<sub>6</sub>, Zn(H<sub>2</sub>O)<sub>6</sub>TiF<sub>6</sub>, Zn(H<sub>2</sub>O)<sub>6</sub>ZrF<sub>6</sub>

- Ni(H<sub>2</sub>O)<sub>6</sub>SnCl<sub>6</sub> is the prototype for a large class of molecular crystals with the form MG<sub>6</sub>LR<sub>6</sub>, where MG<sub>6</sub> is a cation and LR<sub>6</sub> is an anion. (Hermann, 1937) gave this the *Strukturbericht* designation *I*6<sub>1</sub>. (Gottfried, 1937) changed the *I* designations to *J*, so this should have become *J*6<sub>1</sub>, but it was never referenced in any form in later volumes of *Strukturbericht*. Since *I*6<sub>1</sub> is the only designation for this structure in the literature, we use it rather than *J*1<sub>6</sub>.

### 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) Ni I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(1b) Sn I
$\mathbf{B}_3$	=	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_4$	=	$z_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + y_3 \mathbf{a}_3$	=	$-\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_5$	=	$y_3 \mathbf{a}_1 + z_3 \mathbf{a}_2 + x_3 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} + \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_6$	=	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-\frac{1}{2}a(x_3 - z_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 - 2y_3 + z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_7$	=	$-z_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - y_3 \mathbf{a}_3$	=	$\frac{1}{2}a(y_3 - z_3) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_3 - y_3 - z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_8$	=	$-y_3 \mathbf{a}_1 - z_3 \mathbf{a}_2 - x_3 \mathbf{a}_3$	=	$\frac{1}{2}a(x_3 - y_3) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_3 + y_3 - 2z_3) \hat{\mathbf{y}} - \frac{1}{3}c(x_3 + y_3 + z_3) \hat{\mathbf{z}}$	(6f) Cl I
$\mathbf{B}_9$	=	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}}$	(6f) H I

$$\begin{aligned}
\mathbf{B}_{10} &= z_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + y_4 \mathbf{a}_3 &= -\frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} & (6f) & \text{H I} \\
\mathbf{B}_{11} &= y_4 \mathbf{a}_1 + z_4 \mathbf{a}_2 + x_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} + \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} & (6f) & \text{H I} \\
\mathbf{B}_{12} &= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3 &= -\frac{1}{2}a(x_4 - z_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 - 2y_4 + z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} & (6f) & \text{H I} \\
\mathbf{B}_{13} &= -z_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - y_4 \mathbf{a}_3 &= \frac{1}{2}a(y_4 - z_4) \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a(2x_4 - y_4 - z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} & (6f) & \text{H I} \\
\mathbf{B}_{14} &= -y_4 \mathbf{a}_1 - z_4 \mathbf{a}_2 - x_4 \mathbf{a}_3 &= \frac{1}{2}a(x_4 - y_4) \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a(x_4 + y_4 - 2z_4) \hat{\mathbf{y}} - \frac{1}{3}c(x_4 + y_4 + z_4) \hat{\mathbf{z}} & (6f) & \text{H I}
\end{aligned}$$

## References

- [1] L. Pauling, *On the crystal structure of nickel chlorostannate hexahydrate*, Z. Krystallogr. **72**, 482–492 (1930), doi:10.1524/zkri.1930.72.1.482.
- [2] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

## Found in

- [1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).