# $Sr_2NiTeO_6$ Structure: AB6C2D_mC40_12_ac_gh4i_j_bd-001

This structure originally had the label `AB6C2D_mC40_12_ad_gh4i_j_bc`. Calls to that address will be redirected here.

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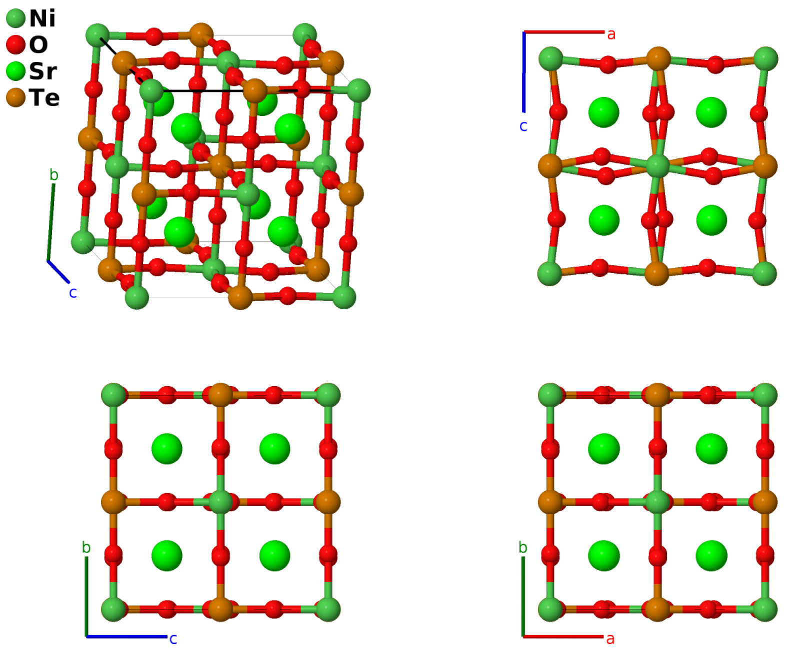
https://aflow.org/p/79Y1

https://aflow.org/p/AB6C2D_mC40_12_ac_gh4i_j_bd-001




| | |
|---|---|
| **Prototype** | $NiO_6Sr_2Te$ |
| **AFLOW prototype label** | AB6C2D_mC40_12_ac_gh4i_j_bd-001 |
| **ICSD** | 91792 |
| **Pearson symbol** | mC40 |
| **Space group number** | 12 |
| **Space group symbol** | $C2/m$ |
| **AFLOW prototype command** | `aflow --proto=AB6C2D_mC40_12_ac_gh4i_j_bd-001`<br>`--params=`$a, b/a, c/a, \beta, y_5, y_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, y_{11}, z_{11}$ |

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**Other compounds with this structure**

$Sr_2NiTeO_6$, $Cs_2RbDy_6$

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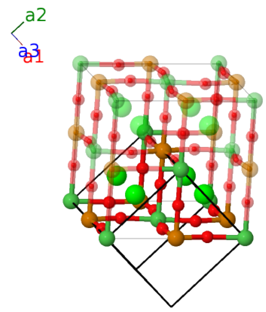
- At high temperatures $Sr_2NiTeO_6$ transforms into the cubic perovskite $E2_1$ structure.

## Base-centered Monoclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} - \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\mathbf{\hat{x}} + \tfrac{1}{2}b\,\mathbf{\hat{y}} \\
\mathbf{a_3} &= c\cos\beta\,\mathbf{\hat{x}} + c\sin\beta\,\mathbf{\hat{z}}
\end{aligned}
$$




## Basis vectors

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | Ni I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$ | = | $\frac{1}{2}a\,\mathbf{\hat{x}}$ | (2b) | Te I |
| $\mathbf{B_3}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\cos\beta\,\mathbf{\hat{x}} + \frac{1}{2}c\sin\beta\,\mathbf{\hat{z}}$ | (2c) | Ni II |
| $\mathbf{B_4}$ | = | $\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}\left(a + c\cos\beta\right)\,\mathbf{\hat{x}} + \frac{1}{2}c\sin\beta\,\mathbf{\hat{z}}$ | (2d) | Te II |
| $\mathbf{B_5}$ | = | $-y_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$ | = | $by_5\,\mathbf{\hat{y}}$ | (4g) | O I |
| $\mathbf{B_6}$ | = | $y_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2$ | = | $-by_5\,\mathbf{\hat{y}}$ | (4g) | O I |
| $\mathbf{B_7}$ | = | $-y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\cos\beta\,\mathbf{\hat{x}} + by_6\,\mathbf{\hat{y}} + \frac{1}{2}c\sin\beta\,\mathbf{\hat{z}}$ | (4h) | O II |
| $\mathbf{B_8}$ | = | $y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\cos\beta\,\mathbf{\hat{x}} - by_6\,\mathbf{\hat{y}} + \frac{1}{2}c\sin\beta\,\mathbf{\hat{z}}$ | (4h) | O II |
| $\mathbf{B_9}$ | = | $x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$ | = | $\left(ax_7 + cz_7\cos\beta\right)\,\mathbf{\hat{x}} + cz_7\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O III |
| $\mathbf{B_{10}}$ | = | $-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$ | = | $-\left(ax_7 + cz_7\cos\beta\right)\,\mathbf{\hat{x}} - cz_7\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O III |
| $\mathbf{B_{11}}$ | = | $x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$ | = | $\left(ax_8 + cz_8\cos\beta\right)\,\mathbf{\hat{x}} + cz_8\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O IV |
| $\mathbf{B_{12}}$ | = | $-x_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$ | = | $-\left(ax_8 + cz_8\cos\beta\right)\,\mathbf{\hat{x}} - cz_8\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O IV |
| $\mathbf{B_{13}}$ | = | $x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$ | = | $\left(ax_9 + cz_9\cos\beta\right)\,\mathbf{\hat{x}} + cz_9\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O V |
| $\mathbf{B_{14}}$ | = | $-x_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$ | = | $-\left(ax_9 + cz_9\cos\beta\right)\,\mathbf{\hat{x}} - cz_9\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O V |
| $\mathbf{B_{15}}$ | = | $x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$ | = | $\left(ax_{10} + cz_{10}\cos\beta\right)\,\mathbf{\hat{x}} + cz_{10}\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O VI |
| $\mathbf{B_{16}}$ | = | $-x_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3$ | = | $-\left(ax_{10} + cz_{10}\cos\beta\right)\,\mathbf{\hat{x}} - cz_{10}\sin\beta\,\mathbf{\hat{z}}$ | (4i) | O VI |
| $\mathbf{B_{17}}$ | = | $\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 + \left(x_{11} + y_{11}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$ | = | $\left(ax_{11} + cz_{11}\cos\beta\right)\,\mathbf{\hat{x}} + by_{11}\,\mathbf{\hat{y}} + cz_{11}\sin\beta\,\mathbf{\hat{z}}$ | (8j) | Sr I |
| $\mathbf{B_{18}}$ | = | $-\left(x_{11} + y_{11}\right)\,\mathbf{a}_1 - \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$ | = | $-\left(ax_{11} + cz_{11}\cos\beta\right)\,\mathbf{\hat{x}} + by_{11}\,\mathbf{\hat{y}} - cz_{11}\sin\beta\,\mathbf{\hat{z}}$ | (8j) | Sr I |
| $\mathbf{B_{19}}$ | = | $-\left(x_{11} - y_{11}\right)\,\mathbf{a}_1 - \left(x_{11} + y_{11}\right)\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3$ | = | $-\left(ax_{11} + cz_{11}\cos\beta\right)\,\mathbf{\hat{x}} - by_{11}\,\mathbf{\hat{y}} - cz_{11}\sin\beta\,\mathbf{\hat{z}}$ | (8j) | Sr I |
| $\mathbf{B_{20}}$ | = | $\left(x_{11} + y_{11}\right)\,\mathbf{a}_1 + \left(x_{11} - y_{11}\right)\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$ | = | $\left(ax_{11} + cz_{11}\cos\beta\right)\,\mathbf{\hat{x}} - by_{11}\,\mathbf{\hat{y}} + cz_{11}\sin\beta\,\mathbf{\hat{z}}$ | (8j) | Sr I |

## References


[1] D. Iwanaga, Y. Inaguma, and M. Itoh, *Structure and Magnetic Properties of $Sr_2NiAO_6$ (A = W, Te)*, Mater. Res. Bull. **35**, 449–457 (2000), doi:10.1016/S0025-5408(00)00222-1.