

Nd₂Te₅ Structure:

A2B5_oC28_63_2c_5c-001

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<https://aflow.org/prototype-encyclopedia/BKM3>

https://aflow.org/prototype-encyclopedia/A2B5_oC28_63_2c_5c-001

Prototype	Nd ₂ Te ₅
AFLOW prototype label	A2B5_oC28_63_2c_5c-001
ICSD	646005
CCDC	1762051
Pearson symbol	oC28
Space group number	63
Space group symbol	<i>Cmcm</i>
AFLOW prototype command	<code>aflow --proto=A2B5_oC28_63_2c_5c-001</code> <code>--params=a, b/a, c/a, y₁, y₂, y₃, y₄, y₅, y₆, y₇</code>

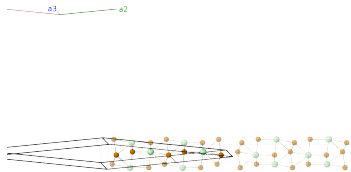
Other compounds with this structure

Ce₂Te₅, Dy₂Te₅, Gd₂Te₅, Ge₂Te₅, Ho₂Te₅, La₂Te₅, Nd₂Te₅, Pr₂Te₅, Sm₂Te₅

- Nd₂Te₅ can also be found in the stibnite (*D*5₈) structure.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

Lattice coordinates	Cartesian coordinates	Wyckoff position	Atom type
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$\mathbf{B}_1$	$=$	$-y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_1 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Nd I
$\mathbf{B}_2$	$=$	$y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_1 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Nd I
$\mathbf{B}_3$	$=$	$-y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_2 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Nd II
$\mathbf{B}_4$	$=$	$y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_2 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Nd II
$\mathbf{B}_5$	$=$	$-y_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_3 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_6$	$=$	$y_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_3 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Te I
$\mathbf{B}_7$	$=$	$-y_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_4 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_8$	$=$	$y_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_4 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Te II
$\mathbf{B}_9$	$=$	$-y_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_5 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Te III
$\mathbf{B}_{10}$	$=$	$y_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_5 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Te III
$\mathbf{B}_{11}$	$=$	$-y_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_6 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Te IV
$\mathbf{B}_{12}$	$=$	$y_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_6 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Te IV
$\mathbf{B}_{13}$	$=$	$-y_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$by_7 \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(4c)	Te V
$\mathbf{B}_{14}$	$=$	$y_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$-by_7 \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(4c)	Te V

References

- [1] M.-P. Pardo and J. Flahaut, *Les tellurures L_2Te_5 des elements des terres rares*, Comptes Rendus des Seances de l'Academie des Sciences, Série C: Sciences Chimiques **263**, 1058–1060 (1966).

Found in

- [1] ICSD, Inorganic Crystal Structure Database. ID 24181.

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Nd
Te

