

α -KHo₂F₇ Structure:

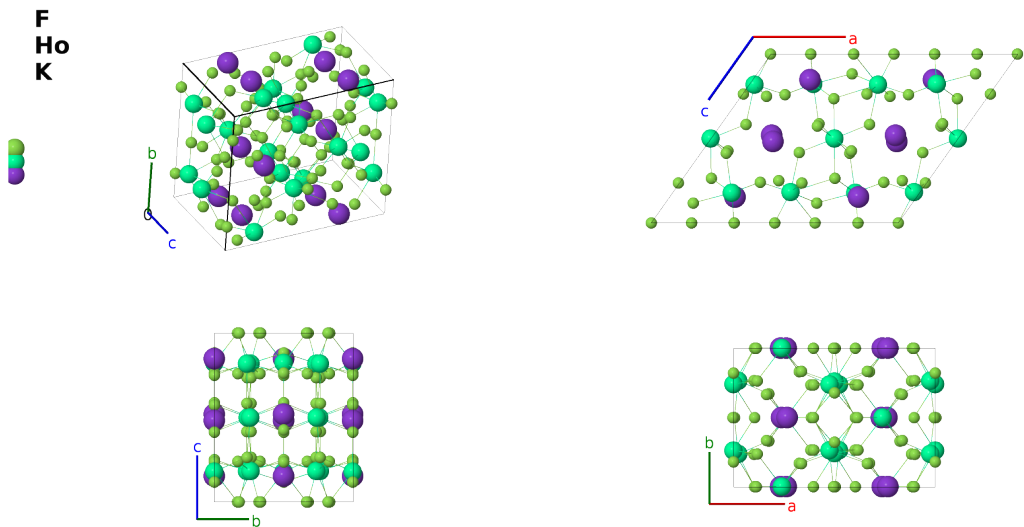
A7B2C_mC80_12_g5i4j_hij_2i-001

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<https://aflow.org/prototype-encyclopedia/C4TT>

https://aflow.org/prototype-encyclopedia/A7B2C_mC80_12_g5i4j_hij_2i-001



Prototype	F ₇ Ho ₂ K
AFLOW prototype label	A7B2C_mC80_12_g5i4j_hij_2i-001
ICSD	63531
CCDC	1626634
Pearson symbol	mC80
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	<pre>aflow --proto=A7B2C_mC80_12_g5i4j_hij_2i-001 --params=a,b/a,c/a,β,y₁,y₂,x₃,z₃,x₄,z₄,x₅,z₅,x₆,z₆,x₇,z₇,x₈,z₈,x₉,z₉,x₁₀,z₁₀, x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅,y₁₅,z₁₅</pre>

Other compounds with this structure

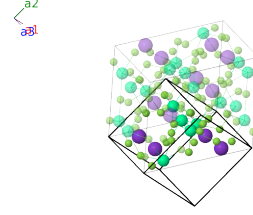
α -KEr₂F₇

- This is the low-temperature structure of KHo₂F₇. At higher temperatures it transforms in to the β -KEr₂F₇ structure.
- (le Fur, 1982) placed this structure in the non-centrosymmetric Cm #8 space group. (Marsh, 1988) found that the structure could be equally well refined in centrosymmetric $C2/m$.

- The default AFLOW parameterization of this structure rather severely distorts the monoclinic unit cell, changing the angle β from 125.33° to 144.257° . Although of course it produces an equivalent structure, we have chosen to use the more compact experimental description of the lattice here.

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
$\mathbf{B}_1$	$= -y_1 \mathbf{a}_1 + y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(4g)	F I
$\mathbf{B}_2$	$= y_1 \mathbf{a}_1 - y_1 \mathbf{a}_2$	$=$	$-by_1 \hat{\mathbf{y}}$	(4g)	F I
$\mathbf{B}_3$	$= -y_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Ho I
$\mathbf{B}_4$	$= y_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(4h)	Ho I
$\mathbf{B}_5$	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	F II
$\mathbf{B}_6$	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i)	F II
$\mathbf{B}_7$	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	F III
$\mathbf{B}_8$	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i)	F III
$\mathbf{B}_9$	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	F IV
$\mathbf{B}_{10}$	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i)	F IV
$\mathbf{B}_{11}$	$= x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	F V
$\mathbf{B}_{12}$	$= -x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i)	F V
$\mathbf{B}_{13}$	$= x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	F VI
$\mathbf{B}_{14}$	$= -x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i)	F VI
$\mathbf{B}_{15}$	$= x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i)	Ho II
$\mathbf{B}_{16}$	$= -x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i)	Ho II
$\mathbf{B}_{17}$	$= x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	K I
$\mathbf{B}_{18}$	$= -x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4i)	K I
$\mathbf{B}_{19}$	$= x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i)	K II
$\mathbf{B}_{20}$	$= -x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i)	K II
$\mathbf{B}_{21}$	$= (x_{11} - y_{11}) \mathbf{a}_1 +$ $(x_{11} + y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	F VII
$\mathbf{B}_{22}$	$= -(x_{11} + y_{11}) \mathbf{a}_1 -$ $(x_{11} - y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} -$ $cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	F VII
$\mathbf{B}_{23}$	$= -(x_{11} - y_{11}) \mathbf{a}_1 -$ $(x_{11} + y_{11}) \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} -$ $cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	F VII
$\mathbf{B}_{24}$	$= (x_{11} + y_{11}) \mathbf{a}_1 +$ $(x_{11} - y_{11}) \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - by_{11} \hat{\mathbf{y}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(8j)	F VII

$\mathbf{B}_{25} =$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	F VIII
$\mathbf{B}_{26} =$	$-(x_{12} + y_{12}) \mathbf{a}_1 -$ $(x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	F VIII
$\mathbf{B}_{27} =$	$-(x_{12} - y_{12}) \mathbf{a}_1 -$ $(x_{12} + y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	F VIII
$\mathbf{B}_{28} =$	$(x_{12} + y_{12}) \mathbf{a}_1 +$ $(x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j)	F VIII
$\mathbf{B}_{29} =$	$(x_{13} - y_{13}) \mathbf{a}_1 +$ $(x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	F IX
$\mathbf{B}_{30} =$	$-(x_{13} + y_{13}) \mathbf{a}_1 -$ $(x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	F IX
$\mathbf{B}_{31} =$	$-(x_{13} - y_{13}) \mathbf{a}_1 -$ $(x_{13} + y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	F IX
$\mathbf{B}_{32} =$	$(x_{13} + y_{13}) \mathbf{a}_1 +$ $(x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j)	F IX
$\mathbf{B}_{33} =$	$(x_{14} - y_{14}) \mathbf{a}_1 +$ $(x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	F X
$\mathbf{B}_{34} =$	$-(x_{14} + y_{14}) \mathbf{a}_1 -$ $(x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} -$ $cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	F X
$\mathbf{B}_{35} =$	$-(x_{14} - y_{14}) \mathbf{a}_1 -$ $(x_{14} + y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} -$ $cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	F X
$\mathbf{B}_{36} =$	$(x_{14} + y_{14}) \mathbf{a}_1 +$ $(x_{14} - y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	F X
$\mathbf{B}_{37} =$	$(x_{15} - y_{15}) \mathbf{a}_1 +$ $(x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Ho III
$\mathbf{B}_{38} =$	$-(x_{15} + y_{15}) \mathbf{a}_1 -$ $(x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} -$ $cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Ho III
$\mathbf{B}_{39} =$	$-(x_{15} - y_{15}) \mathbf{a}_1 -$ $(x_{15} + y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} -$ $cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Ho III
$\mathbf{B}_{40} =$	$(x_{15} + y_{15}) \mathbf{a}_1 +$ $(x_{15} - y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Ho III

References

- [1] R. E. Marsh and F. Herstein, *More space-group changes* **44**, 77–88 (1988), doi:10.1107/S0108768187009492.
- [2] Y. L. Fur, S. Aléonard, M. F. Gorius, and M. T. Roux, *Structure des phases de type α -K Er_2F_7* **38**, 1431–1436 (1982), doi:10.1107/S0567740882006098.

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