

Al₄₅V₇ Structure:

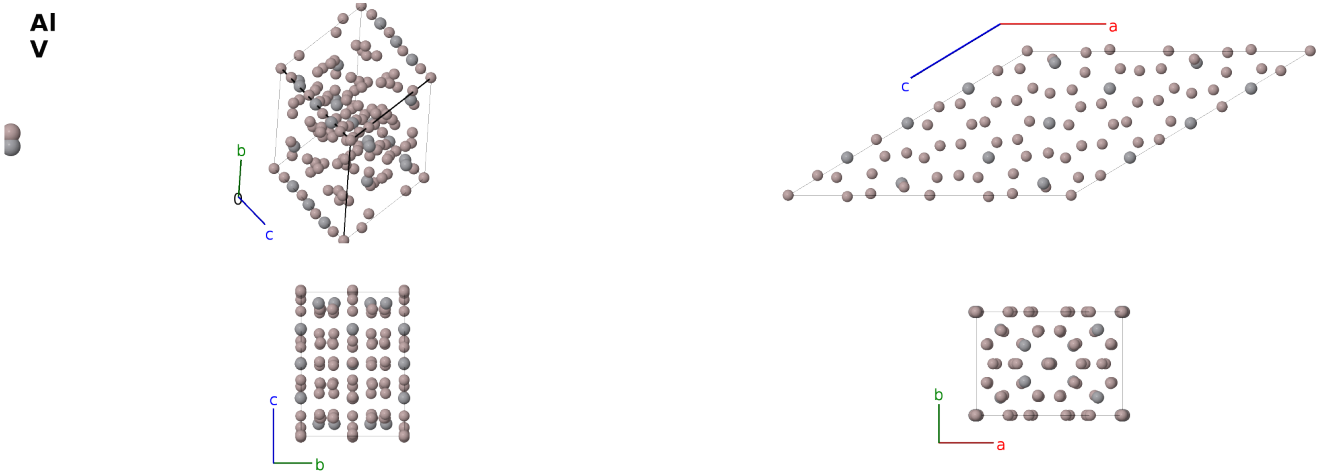
A45B7_mC104_12_a8i7j_cij-001

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- 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/prototype-encyclopedia/4Z2U>

https://aflow.org/prototype-encyclopedia/A45B7_mC104_12_a8i7j_cij-001



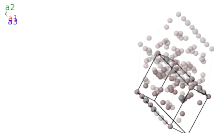
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ICSD	58204
CCDC	1622232
Pearson symbol	mC104
Space group number	12
Space group symbol	C2/m
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Other compounds with this structure

Al₄₅Cr₇

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
$\mathbf{B}_1$	$=$	0	$=$	0	(2a) Al I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2c) V I
$\mathbf{B}_3$	$=$	$x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al II
$\mathbf{B}_4$	$=$	$-x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4i) Al II
$\mathbf{B}_5$	$=$	$x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_6$	$=$	$-x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4i) Al III
$\mathbf{B}_7$	$=$	$x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_8$	$=$	$-x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4i) Al IV
$\mathbf{B}_9$	$=$	$x_6 \mathbf{a}_1 + x_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Al V
$\mathbf{B}_{10}$	$=$	$-x_6 \mathbf{a}_1 - x_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4i) Al V
$\mathbf{B}_{11}$	$=$	$x_7 \mathbf{a}_1 + x_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Al VI
$\mathbf{B}_{12}$	$=$	$-x_7 \mathbf{a}_1 - x_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(4i) Al VI
$\mathbf{B}_{13}$	$=$	$x_8 \mathbf{a}_1 + x_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Al VII
$\mathbf{B}_{14}$	$=$	$-x_8 \mathbf{a}_1 - x_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(4i) Al VII
$\mathbf{B}_{15}$	$=$	$x_9 \mathbf{a}_1 + x_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(4i) Al VIII
$\mathbf{B}_{16}$	$=$	$-x_9 \mathbf{a}_1 - x_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(4i) Al VIII
$\mathbf{B}_{17}$	$=$	$x_{10} \mathbf{a}_1 + x_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i) Al IX
$\mathbf{B}_{18}$	$=$	$-x_{10} \mathbf{a}_1 - x_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(4i) Al IX
$\mathbf{B}_{19}$	$=$	$x_{11} \mathbf{a}_1 + x_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} + cz_{11} \sin \beta \hat{\mathbf{z}}$	(4i) V II
$\mathbf{B}_{20}$	$=$	$-x_{11} \mathbf{a}_1 - x_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3$	$=$	$-(ax_{11} + cz_{11} \cos \beta) \hat{\mathbf{x}} - cz_{11} \sin \beta \hat{\mathbf{z}}$	(4i) V II
$\mathbf{B}_{21}$	$=$	$(x_{12} - y_{12}) \mathbf{a}_1 +$ $(x_{12} + y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Al X
$\mathbf{B}_{22}$	$=$	$-(x_{12} + y_{12}) \mathbf{a}_1 -$ $(x_{12} - y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Al X
$\mathbf{B}_{23}$	$=$	$-(x_{12} - y_{12}) \mathbf{a}_1 -$ $(x_{12} + y_{12}) \mathbf{a}_2 - z_{12} \mathbf{a}_3$	$=$	$-(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} -$ $cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Al X
$\mathbf{B}_{24}$	$=$	$(x_{12} + y_{12}) \mathbf{a}_1 +$ $(x_{12} - y_{12}) \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + cz_{12} \cos \beta) \hat{\mathbf{x}} - by_{12} \hat{\mathbf{y}} + cz_{12} \sin \beta \hat{\mathbf{z}}$	(8j) Al X
$\mathbf{B}_{25}$	$=$	$(x_{13} - y_{13}) \mathbf{a}_1 +$ $(x_{13} + y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j) Al XI
$\mathbf{B}_{26}$	$=$	$-(x_{13} + y_{13}) \mathbf{a}_1 -$ $(x_{13} - y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j) Al XI
$\mathbf{B}_{27}$	$=$	$-(x_{13} - y_{13}) \mathbf{a}_1 -$ $(x_{13} + y_{13}) \mathbf{a}_2 - z_{13} \mathbf{a}_3$	$=$	$-(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} -$ $cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j) Al XI
$\mathbf{B}_{28}$	$=$	$(x_{13} + y_{13}) \mathbf{a}_1 +$ $(x_{13} - y_{13}) \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} + cz_{13} \sin \beta \hat{\mathbf{z}}$	(8j) Al XI
$\mathbf{B}_{29}$	$=$	$(x_{14} - y_{14}) \mathbf{a}_1 +$ $(x_{14} + y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j) Al XII
$\mathbf{B}_{30}$	$=$	$-(x_{14} + y_{14}) \mathbf{a}_1 -$ $(x_{14} - y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} -$ $cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j) Al XII

$\mathbf{B}_{31} =$	$-(x_{14} - y_{14}) \mathbf{a}_1 -$ $(x_{14} + y_{14}) \mathbf{a}_2 - z_{14} \mathbf{a}_3$	$=$	$-(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} -$ $cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XII
$\mathbf{B}_{32} =$	$(x_{14} + y_{14}) \mathbf{a}_1 +$ $(x_{14} - y_{14}) \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XII
$\mathbf{B}_{33} =$	$(x_{15} - y_{15}) \mathbf{a}_1 +$ $(x_{15} + y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B}_{34} =$	$-(x_{15} + y_{15}) \mathbf{a}_1 -$ $(x_{15} - y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}} -$ $cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B}_{35} =$	$-(x_{15} - y_{15}) \mathbf{a}_1 -$ $(x_{15} + y_{15}) \mathbf{a}_2 - z_{15} \mathbf{a}_3$	$=$	$-(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} -$ $cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B}_{36} =$	$(x_{15} + y_{15}) \mathbf{a}_1 +$ $(x_{15} - y_{15}) \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + cz_{15} \cos \beta) \hat{\mathbf{x}} - by_{15} \hat{\mathbf{y}} + cz_{15} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIII
$\mathbf{B}_{37} =$	$(x_{16} - y_{16}) \mathbf{a}_1 +$ $(x_{16} + y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B}_{38} =$	$-(x_{16} + y_{16}) \mathbf{a}_1 -$ $(x_{16} - y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} -$ $cz_{16} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B}_{39} =$	$-(x_{16} - y_{16}) \mathbf{a}_1 -$ $(x_{16} + y_{16}) \mathbf{a}_2 - z_{16} \mathbf{a}_3$	$=$	$-(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} -$ $cz_{16} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B}_{40} =$	$(x_{16} + y_{16}) \mathbf{a}_1 +$ $(x_{16} - y_{16}) \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + cz_{16} \cos \beta) \hat{\mathbf{x}} - by_{16} \hat{\mathbf{y}} + cz_{16} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XIV
$\mathbf{B}_{41} =$	$(x_{17} - y_{17}) \mathbf{a}_1 +$ $(x_{17} + y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B}_{42} =$	$-(x_{17} + y_{17}) \mathbf{a}_1 -$ $(x_{17} - y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} -$ $cz_{17} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B}_{43} =$	$-(x_{17} - y_{17}) \mathbf{a}_1 -$ $(x_{17} + y_{17}) \mathbf{a}_2 - z_{17} \mathbf{a}_3$	$=$	$-(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} -$ $cz_{17} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B}_{44} =$	$(x_{17} + y_{17}) \mathbf{a}_1 +$ $(x_{17} - y_{17}) \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + cz_{17} \cos \beta) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + cz_{17} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XV
$\mathbf{B}_{45} =$	$(x_{18} - y_{18}) \mathbf{a}_1 +$ $(x_{18} + y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B}_{46} =$	$-(x_{18} + y_{18}) \mathbf{a}_1 -$ $(x_{18} - y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} -$ $cz_{18} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B}_{47} =$	$-(x_{18} - y_{18}) \mathbf{a}_1 -$ $(x_{18} + y_{18}) \mathbf{a}_2 - z_{18} \mathbf{a}_3$	$=$	$-(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} -$ $cz_{18} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B}_{48} =$	$(x_{18} + y_{18}) \mathbf{a}_1 +$ $(x_{18} - y_{18}) \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + cz_{18} \cos \beta) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + cz_{18} \sin \beta \hat{\mathbf{z}}$	(8j)	Al XVI
$\mathbf{B}_{49} =$	$(x_{19} - y_{19}) \mathbf{a}_1 +$ $(x_{19} + y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{50} =$	$-(x_{19} + y_{19}) \mathbf{a}_1 -$ $(x_{19} - y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} -$ $cz_{19} \sin \beta \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{51} =$	$-(x_{19} - y_{19}) \mathbf{a}_1 -$ $(x_{19} + y_{19}) \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} -$ $cz_{19} \sin \beta \hat{\mathbf{z}}$	(8j)	V III
$\mathbf{B}_{52} =$	$(x_{19} + y_{19}) \mathbf{a}_1 +$ $(x_{19} - y_{19}) \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(8j)	V III

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