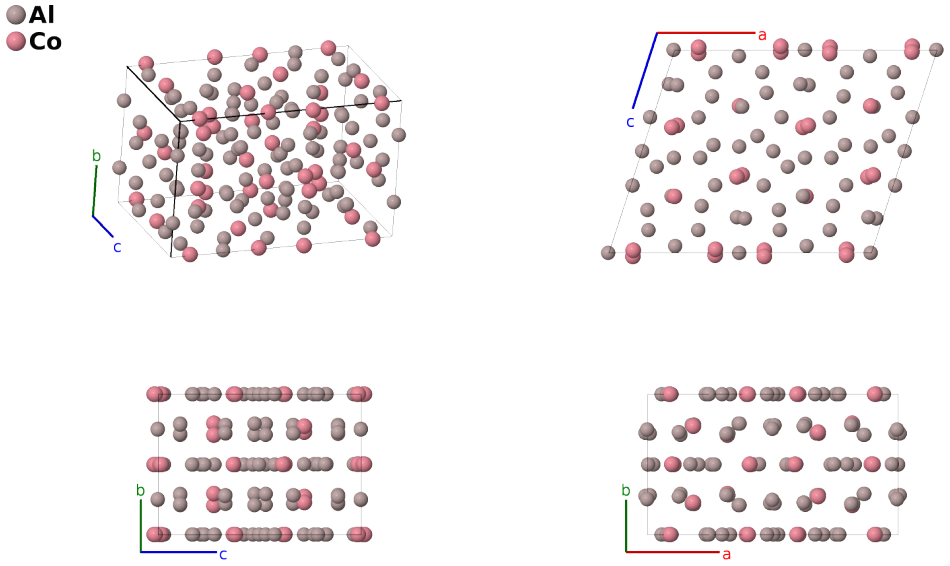
Monoclinic Co_4Al_{13} Structure: A13B4_mC102_8_17a11b_8a2b-001

This structure originally had the label `A13B4_mC102_8_17a11b_8a2b`. 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/DU5A

https://aflow.org/p/A13B4_mC102_8_17a11b_8a2b-001



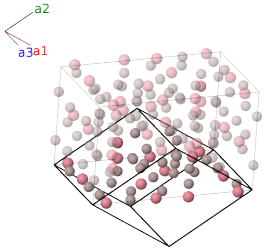
Prototype	$Al_{13}Co_4$
AFLOW prototype label	A13B4_mC102_8_17a11b_8a2b-001
ICSD	57599
Pearson symbol	mC102
Space group number	8
Space group symbol	Cm
AFLOW prototype command	`aflow --proto=A13B4_mC102_8_17a11b_8a2b-001 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3, x_4, z_4, x_5, z_5, x_6, z_6, x_7, z_7, x_8, z_8, x_9, z_9, x_{10}, z_{10}, x_{11}, z_{11}, x_{12}, z_{12}, x_{13}, z_{13}, x_{14}, z_{14}, x_{15}, z_{15}, x_{16}, z_{16}, x_{17}, z_{17}, x_{18}, z_{18}, x_{19}, z_{19}, x_{20}, z_{20}, x_{21}, z_{21}, x_{22}, z_{22}, x_{23}, z_{23}, x_{24}, z_{24}, x_{25}, z_{25}, x_{26}, y_{26}, z_{26}, x_{27}, y_{27}, z_{27}, x_{28}, y_{28}, z_{28}, x_{29}, y_{29}, z_{29}, x_{30}, y_{30}, z_{30}, x_{31}, y_{31}, z_{31}, x_{32}, y_{32}, z_{32}, x_{33}, y_{33}, z_{33}, x_{34}, y_{34}, z_{34}, x_{35}, y_{35}, z_{35}, x_{36}, y_{36}, z_{36}, x_{37}, y_{37}, z_{37}, x_{38}, y_{38}, z_{38}$

- Following (Hudd, 1962), the Al-IV and Al-XIII sites are occupied 30% of the time, while the occupation of Al-VI, Al-IX, Al-XIV, and Al-XVII is 70%. This gives a nominal occupation of $Al_{91}Co_{30}$, though the authors state the actual composition is $Al_{68.3}Co_{24.4}$.
- Space group Cm #8 allows an arbitrary choice for the origin of the z-axis. We follow (Hudd, 1962) and set $z_{26} = 0$.

- If we allow the rather large uncertainty of 0.3Å in the atomic positions, FINDSYM sets the symmetry as $C2/m$ #12. That crystal has the $Al_{13}Fe_4$ prototype.
- Co_4 has also been observed in a orthorhombic structure.

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al III
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al IV
$\mathbf{B_5}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al V
$\mathbf{B_6}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al VI
$\mathbf{B_7}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al VII
$\mathbf{B_8}$	=	$x_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al VIII
$\mathbf{B_9}$	=	$x_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al IX
$\mathbf{B_{10}}$	=	$x_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + cz_{10}\cos\beta)\,\hat{\mathbf{x}} + cz_{10}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al X
$\mathbf{B_{11}}$	=	$x_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3$	=	$(ax_{11} + cz_{11}\cos\beta)\,\hat{\mathbf{x}} + cz_{11}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XI
$\mathbf{B_{12}}$	=	$x_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3$	=	$(ax_{12} + cz_{12}\cos\beta)\,\hat{\mathbf{x}} + cz_{12}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XII
$\mathbf{B_{13}}$	=	$x_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3$	=	$(ax_{13} + cz_{13}\cos\beta)\,\hat{\mathbf{x}} + cz_{13}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XIII
$\mathbf{B_{14}}$	=	$x_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3$	=	$(ax_{14} + cz_{14}\cos\beta)\,\hat{\mathbf{x}} + cz_{14}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XIV
$\mathbf{B_{15}}$	=	$x_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3$	=	$(ax_{15} + cz_{15}\cos\beta)\,\hat{\mathbf{x}} + cz_{15}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XV
$\mathbf{B_{16}}$	=	$x_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3$	=	$(ax_{16} + cz_{16}\cos\beta)\,\hat{\mathbf{x}} + cz_{16}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XVI
$\mathbf{B_{17}}$	=	$x_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3$	=	$(ax_{17} + cz_{17}\cos\beta)\,\hat{\mathbf{x}} + cz_{17}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Al XVII
$\mathbf{B_{18}}$	=	$x_{18}\,\mathbf{a}_1 + x_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3$	=	$(ax_{18} + cz_{18}\cos\beta)\,\hat{\mathbf{x}} + cz_{18}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co I
$\mathbf{B_{19}}$	=	$x_{19}\,\mathbf{a}_1 + x_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3$	=	$(ax_{19} + cz_{19}\cos\beta)\,\hat{\mathbf{x}} + cz_{19}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co II
$\mathbf{B_{20}}$	=	$x_{20}\,\mathbf{a}_1 + x_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$(ax_{20} + cz_{20}\cos\beta)\,\hat{\mathbf{x}} + cz_{20}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co III
$\mathbf{B_{21}}$	=	$x_{21}\,\mathbf{a}_1 + x_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$(ax_{21} + cz_{21}\cos\beta)\,\hat{\mathbf{x}} + cz_{21}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co IV
$\mathbf{B_{22}}$	=	$x_{22}\,\mathbf{a}_1 + x_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$(ax_{22} + cz_{22}\cos\beta)\,\hat{\mathbf{x}} + cz_{22}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co V
$\mathbf{B_{23}}$	=	$x_{23}\,\mathbf{a}_1 + x_{23}\,\mathbf{a}_2 + z_{23}\,\mathbf{a}_3$	=	$(ax_{23} + cz_{23}\cos\beta)\,\hat{\mathbf{x}} + cz_{23}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co VI
$\mathbf{B_{24}}$	=	$x_{24}\,\mathbf{a}_1 + x_{24}\,\mathbf{a}_2 + z_{24}\,\mathbf{a}_3$	=	$(ax_{24} + cz_{24}\cos\beta)\,\hat{\mathbf{x}} + cz_{24}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co VII
$\mathbf{B_{25}}$	=	$x_{25}\,\mathbf{a}_1 + x_{25}\,\mathbf{a}_2 + z_{25}\,\mathbf{a}_3$	=	$(ax_{25} + cz_{25}\cos\beta)\,\hat{\mathbf{x}} + cz_{25}\sin\beta\,\hat{\mathbf{z}}$	(2a)	Co VIII
$\mathbf{B_{26}}$	=	$(x_{26} - y_{26})\,\mathbf{a}_1 + (x_{26} + y_{26})\,\mathbf{a}_2 + z_{26}\,\mathbf{a}_3$	=	$(ax_{26} + cz_{26}\cos\beta)\,\hat{\mathbf{x}} + by_{26}\,\hat{\mathbf{y}} + cz_{26}\sin\beta\,\hat{\mathbf{z}}$	(4b)	Al XVIII

$$\mathbf{B_{27}} = (x_{26}+y_{26})\,\mathbf{a}_1 + (x_{26}-y_{26})\,\mathbf{a}_2 + z_{26}\,\mathbf{a}_3 = (ax_{26}+cz_{26}\cos\beta)\,\hat{\mathbf{x}} - by_{26}\,\hat{\mathbf{y}} + cz_{26}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XVIII}$$

$$\mathbf{B_{28}} = (x_{27}-y_{27})\,\mathbf{a}_1 + (x_{27}+y_{27})\,\mathbf{a}_2 + z_{27}\,\mathbf{a}_3 = (ax_{27}+cz_{27}\cos\beta)\,\hat{\mathbf{x}} + by_{27}\,\hat{\mathbf{y}} + cz_{27}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XIX}$$

$$\mathbf{B_{29}} = (x_{27}+y_{27})\,\mathbf{a}_1 + (x_{27}-y_{27})\,\mathbf{a}_2 + z_{27}\,\mathbf{a}_3 = (ax_{27}+cz_{27}\cos\beta)\,\hat{\mathbf{x}} - by_{27}\,\hat{\mathbf{y}} + cz_{27}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XIX}$$

$$\mathbf{B_{30}} = (x_{28}-y_{28})\,\mathbf{a}_1 + (x_{28}+y_{28})\,\mathbf{a}_2 + z_{28}\,\mathbf{a}_3 = (ax_{28}+cz_{28}\cos\beta)\,\hat{\mathbf{x}} + by_{28}\,\hat{\mathbf{y}} + cz_{28}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XX}$$

$$\mathbf{B_{31}} = (x_{28}+y_{28})\,\mathbf{a}_1 + (x_{28}-y_{28})\,\mathbf{a}_2 + z_{28}\,\mathbf{a}_3 = (ax_{28}+cz_{28}\cos\beta)\,\hat{\mathbf{x}} - by_{28}\,\hat{\mathbf{y}} + cz_{28}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XX}$$

$$\mathbf{B_{32}} = (x_{29}-y_{29})\,\mathbf{a}_1 + (x_{29}+y_{29})\,\mathbf{a}_2 + z_{29}\,\mathbf{a}_3 = (ax_{29}+cz_{29}\cos\beta)\,\hat{\mathbf{x}} + by_{29}\,\hat{\mathbf{y}} + cz_{29}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXI}$$

$$\mathbf{B_{33}} = (x_{29}+y_{29})\,\mathbf{a}_1 + (x_{29}-y_{29})\,\mathbf{a}_2 + z_{29}\,\mathbf{a}_3 = (ax_{29}+cz_{29}\cos\beta)\,\hat{\mathbf{x}} - by_{29}\,\hat{\mathbf{y}} + cz_{29}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXI}$$

$$\mathbf{B_{34}} = (x_{30}-y_{30})\,\mathbf{a}_1 + (x_{30}+y_{30})\,\mathbf{a}_2 + z_{30}\,\mathbf{a}_3 = (ax_{30}+cz_{30}\cos\beta)\,\hat{\mathbf{x}} + by_{30}\,\hat{\mathbf{y}} + cz_{30}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXII}$$

$$\mathbf{B_{35}} = (x_{30}+y_{30})\,\mathbf{a}_1 + (x_{30}-y_{30})\,\mathbf{a}_2 + z_{30}\,\mathbf{a}_3 = (ax_{30}+cz_{30}\cos\beta)\,\hat{\mathbf{x}} - by_{30}\,\hat{\mathbf{y}} + cz_{30}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXII}$$

$$\mathbf{B_{36}} = (x_{31}-y_{31})\,\mathbf{a}_1 + (x_{31}+y_{31})\,\mathbf{a}_2 + z_{31}\,\mathbf{a}_3 = (ax_{31}+cz_{31}\cos\beta)\,\hat{\mathbf{x}} + by_{31}\,\hat{\mathbf{y}} + cz_{31}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXIII}$$

$$\mathbf{B_{37}} = (x_{31}+y_{31})\,\mathbf{a}_1 + (x_{31}-y_{31})\,\mathbf{a}_2 + z_{31}\,\mathbf{a}_3 = (ax_{31}+cz_{31}\cos\beta)\,\hat{\mathbf{x}} - by_{31}\,\hat{\mathbf{y}} + cz_{31}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXIII}$$

$$\mathbf{B_{38}} = (x_{32}-y_{32})\,\mathbf{a}_1 + (x_{32}+y_{32})\,\mathbf{a}_2 + z_{32}\,\mathbf{a}_3 = (ax_{32}+cz_{32}\cos\beta)\,\hat{\mathbf{x}} + by_{32}\,\hat{\mathbf{y}} + cz_{32}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXIV}$$

$$\mathbf{B_{39}} = (x_{32}+y_{32})\,\mathbf{a}_1 + (x_{32}-y_{32})\,\mathbf{a}_2 + z_{32}\,\mathbf{a}_3 = (ax_{32}+cz_{32}\cos\beta)\,\hat{\mathbf{x}} - by_{32}\,\hat{\mathbf{y}} + cz_{32}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXIV}$$

$$\mathbf{B_{40}} = (x_{33}-y_{33})\,\mathbf{a}_1 + (x_{33}+y_{33})\,\mathbf{a}_2 + z_{33}\,\mathbf{a}_3 = (ax_{33}+cz_{33}\cos\beta)\,\hat{\mathbf{x}} + by_{33}\,\hat{\mathbf{y}} + cz_{33}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXV}$$

$$\mathbf{B_{41}} = (x_{33}+y_{33})\,\mathbf{a}_1 + (x_{33}-y_{33})\,\mathbf{a}_2 + z_{33}\,\mathbf{a}_3 = (ax_{33}+cz_{33}\cos\beta)\,\hat{\mathbf{x}} - by_{33}\,\hat{\mathbf{y}} + cz_{33}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXV}$$

$$\mathbf{B_{42}} = (x_{34}-y_{34})\,\mathbf{a}_1 + (x_{34}+y_{34})\,\mathbf{a}_2 + z_{34}\,\mathbf{a}_3 = (ax_{34}+cz_{34}\cos\beta)\,\hat{\mathbf{x}} + by_{34}\,\hat{\mathbf{y}} + cz_{34}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVI}$$

$$\mathbf{B_{43}} = (x_{34}+y_{34})\,\mathbf{a}_1 + (x_{34}-y_{34})\,\mathbf{a}_2 + z_{34}\,\mathbf{a}_3 = (ax_{34}+cz_{34}\cos\beta)\,\hat{\mathbf{x}} - by_{34}\,\hat{\mathbf{y}} + cz_{34}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVI}$$

$$\mathbf{B_{44}} = (x_{35}-y_{35})\,\mathbf{a}_1 + (x_{35}+y_{35})\,\mathbf{a}_2 + z_{35}\,\mathbf{a}_3 = (ax_{35}+cz_{35}\cos\beta)\,\hat{\mathbf{x}} + by_{35}\,\hat{\mathbf{y}} + cz_{35}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVII}$$

$$\mathbf{B_{45}} = (x_{35}+y_{35})\,\mathbf{a}_1 + (x_{35}-y_{35})\,\mathbf{a}_2 + z_{35}\,\mathbf{a}_3 = (ax_{35}+cz_{35}\cos\beta)\,\hat{\mathbf{x}} - by_{35}\,\hat{\mathbf{y}} + cz_{35}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVII}$$

$$\mathbf{B_{46}} = (x_{36}-y_{36})\,\mathbf{a}_1 + (x_{36}+y_{36})\,\mathbf{a}_2 + z_{36}\,\mathbf{a}_3 = (ax_{36}+cz_{36}\cos\beta)\,\hat{\mathbf{x}} + by_{36}\,\hat{\mathbf{y}} + cz_{36}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVIII}$$

$$\mathbf{B_{47}} = (x_{36}+y_{36})\,\mathbf{a}_1 + (x_{36}-y_{36})\,\mathbf{a}_2 + z_{36}\,\mathbf{a}_3 = (ax_{36}+cz_{36}\cos\beta)\,\hat{\mathbf{x}} - by_{36}\,\hat{\mathbf{y}} + cz_{36}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Al XXVIII}$$

$$\mathbf{B_{48}} = (x_{37}-y_{37})\,\mathbf{a}_1 + (x_{37}+y_{37})\,\mathbf{a}_2 + z_{37}\,\mathbf{a}_3 = (ax_{37}+cz_{37}\cos\beta)\,\hat{\mathbf{x}} + by_{37}\,\hat{\mathbf{y}} + cz_{37}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Co IX}$$

$$\mathbf{B_{49}} = (x_{37}+y_{37})\,\mathbf{a}_1 + (x_{37}-y_{37})\,\mathbf{a}_2 + z_{37}\,\mathbf{a}_3 = (ax_{37}+cz_{37}\cos\beta)\,\hat{\mathbf{x}} - by_{37}\,\hat{\mathbf{y}} + cz_{37}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Co IX}$$

$$\mathbf{B_{50}} = (x_{38}-y_{38})\,\mathbf{a}_1 + (x_{38}+y_{38})\,\mathbf{a}_2 + z_{38}\,\mathbf{a}_3 = (ax_{38}+cz_{38}\cos\beta)\,\hat{\mathbf{x}} + by_{38}\,\hat{\mathbf{y}} + cz_{38}\sin\beta\,\hat{\mathbf{z}} \quad (4b) \quad \text{Co X}$$

$\mathbf{B_{51}}$	$= (x_{38} + y_{38})\ \mathbf{a}_1 + (x_{38} - y_{38})\ \mathbf{a}_2 + z_{38}\ \mathbf{a}_3$	$= (ax_{38} + cz_{38}\cos\beta)\ \hat{\mathbf{x}} - by_{38}\ \hat{\mathbf{y}} + cz_{38}\sin\beta\ \hat{\mathbf{z}}$	(4b)	Co X

References

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