Indialite $(K_{0.12}[Fe_2][Mg_{0.85}Fe_{0.15}]_2Al_3 \cdot (Al,Si)_3(Si,Al)_{12}O_{36}$ Structure:

A3BCDE18F6_hP60_177_fg_c_e_d_3n_n-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.

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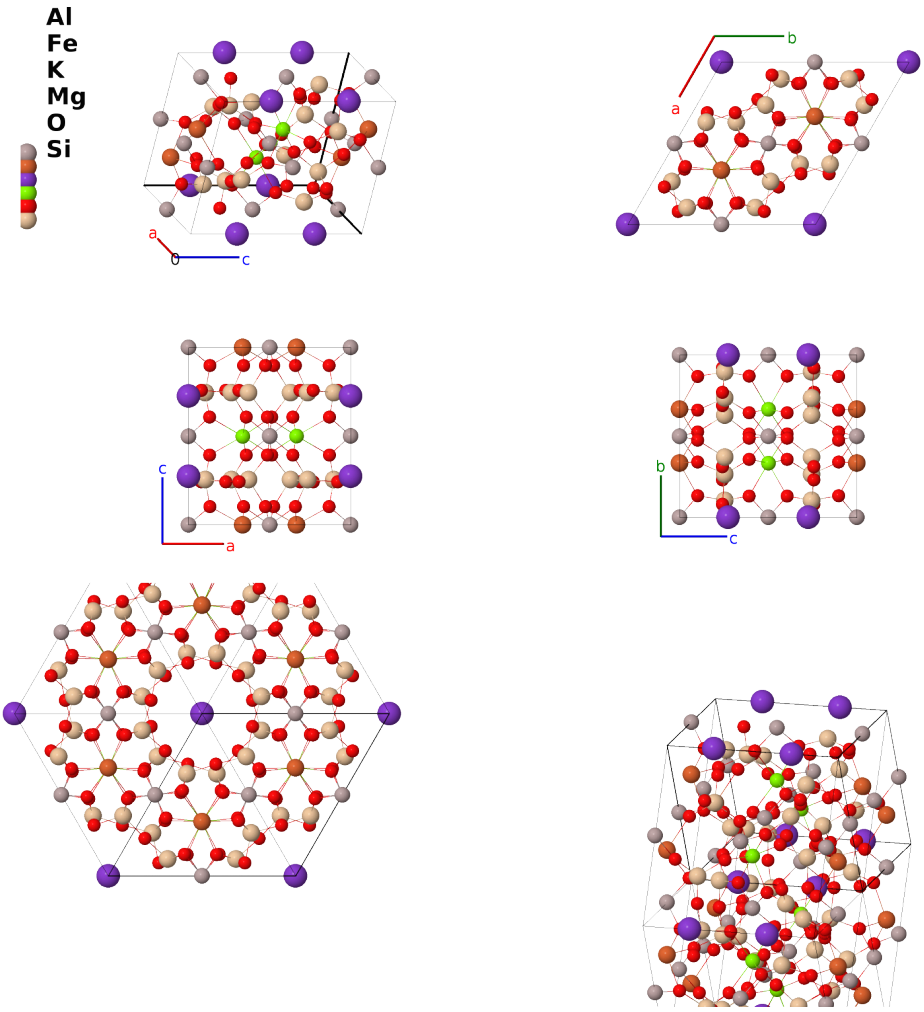
https://aflow.org/prototype-encyclopedia/NUES

https://aflow.org/prototype-encyclopedia/A3BCDE18F6_hP60_177_fg_c_e_d_3n_n-001



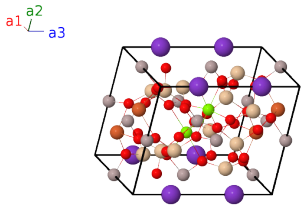
Prototype	$Al_3FeKMgO_{18}S_6$
AFLOW prototype label	A3BCDE18F6_hP60_177_fg_c_e_d_3n_n-001
ICSD	248732
CCDC	1715168
Pearson symbol	hP60

Space group number	177
Space group symbol	$P622$
AFLOW prototype command	`aflow --proto=A3BCDE18F6_hP60_177_fg_c_e_d_3n_n-001 --params=`$a, c/a, z_3, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

- (Rastsvetaeva, 2014) calls this a Fe-analogue of Indialite, and the first mineral to be found in space group $P622$ #177.
- The Mg (2d) site is 85% Mg and 15% Fe. The K (2e) site is only 6% K, and the Si (12n) site is 70% Si and 30% Al, giving the final stoichiometry listed in the title. The ICSD lists three other structures in $P622$, all are equally complicated.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Fe I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(2c)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Mg I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2d)	Mg I
$\mathbf{B_5}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_6}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}}$	(3f)	Al I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(3f)	Al I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3g)	Al II
$\mathbf{B_{13}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{14}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{15}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{16}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{17}}$	=	$y_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{18}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{19}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{20}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{21}}$	=	$-x_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I

$\mathbf{B_{22}}$	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_6+y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6-y_6)\;\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{23}}$	$-\,(x_6-y_6)\;\mathbf{a}_1 + y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_6+2y_6)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{24}}$	$x_6\,\mathbf{a}_1 + (x_6-y_6)\;\mathbf{a}_2 - z_6\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_6-y_6)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(12n)	O I
$\mathbf{B_{25}}$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{26}}$	$-y_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{27}}$	$-\,(x_7-y_7)\;\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{28}}$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{29}}$	$y_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{30}}$	$(x_7-y_7)\;\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{31}}$	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{32}}$	$(x_7-y_7)\;\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_7-2y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{33}}$	$-x_7\,\mathbf{a}_1 - (x_7-y_7)\;\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{34}}$	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_7+y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7-y_7)\;\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{35}}$	$-\,(x_7-y_7)\;\mathbf{a}_1 + y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_7+2y_7)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{36}}$	$x_7\,\mathbf{a}_1 + (x_7-y_7)\;\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_7-y_7)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(12n)	O II
$\mathbf{B_{37}}$	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{38}}$	$-y_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{39}}$	$-\,(x_8-y_8)\;\mathbf{a}_1 - x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{40}}$	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{41}}$	$y_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{42}}$	$(x_8-y_8)\;\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{43}}$	$y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{44}}$	$(x_8-y_8)\;\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_8-2y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{45}}$	$-x_8\,\mathbf{a}_1 - (x_8-y_8)\;\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{46}}$	$-y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_8+y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_8-y_8)\;\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{47}}$	$-\,(x_8-y_8)\;\mathbf{a}_1 + y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_8+2y_8)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{48}}$	$x_8\,\mathbf{a}_1 + (x_8-y_8)\;\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_8-y_8)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(12n)	O III
$\mathbf{B_{49}}$	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{50}}$	$-y_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{51}}$	$-\,(x_9-y_9)\;\mathbf{a}_1 - x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{52}}$	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{53}}$	$y_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{54}}$	$(x_9-y_9)\;\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{55}}$	$y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{56}}$	$(x_9-y_9)\;\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(x_9-2y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{57}}$	$-x_9\,\mathbf{a}_1 - (x_9-y_9)\;\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{58}}$	$-y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$-\frac{1}{2}a\,(x_9+y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_9-y_9)\;\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{59}}$	$-\,(x_9-y_9)\;\mathbf{a}_1 + y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(-x_9+2y_9)\;\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I
$\mathbf{B_{60}}$	$x_9\,\mathbf{a}_1 + (x_9-y_9)\;\mathbf{a}_2 - z_9\,\mathbf{a}_3$	$=$	$\frac{1}{2}a\,(2x_9-y_9)\;\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(12n)	Si I

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[1] R. K. Rastsvetaeva, *Ordered structure of the Fe-analogue of indialite—the first mineral with space group P622*, Doklady Chem. **455**, 62–64 (2014), doi:10.1134/S0012500814050024. First published in Doklady Akademii Nauk 455(5), 544-6 (2014).

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[1] *Inorganic Crystal Structure Database*. Entry 248732 [(Mg0.85 Fe0.15)2 Al3 (Si0.5 Al0.5)3 (Si0.7 Al0.3)12 O36].

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