$MgCuAl_2$ ($E1_a$) Structure: A2BC_oC16_63_f_c_c-002

This structure originally had the label `A2BC_oC16_63_f_c_c`. Calls to that address will be redirected here.

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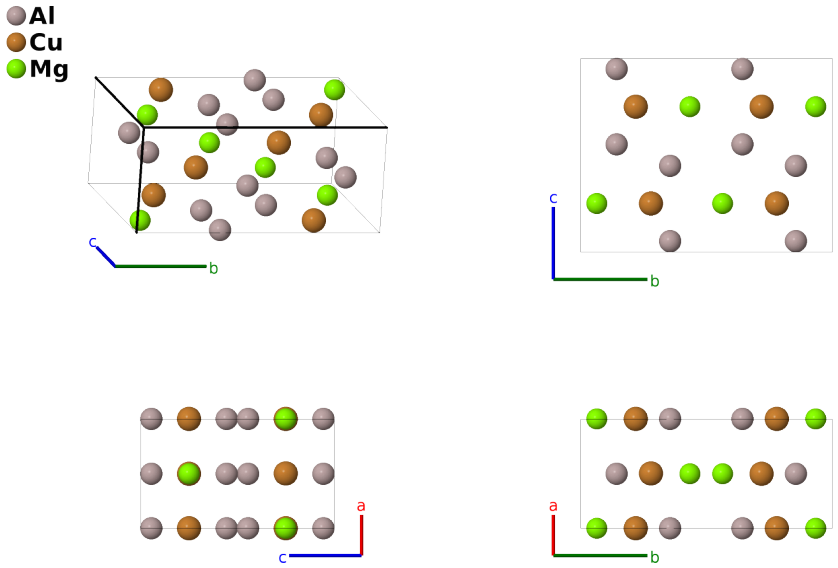
https://aflow.org/p/ECJE

https://aflow.org/p/A2BC_oC16_63_f_c_c-002



Prototype	Al_2CuMg
AFLOW prototype label	A2BC_oC16_63_f_c_c-002
***Strukturbericht* designation**	$E1_a$
ICSD	415062
Pearson symbol	oC16
Space group number	63
Space group symbol	$Cmcm$
AFLOW prototype command	`aflow --proto=A2BC_oC16_63_f_c_c-002 --params=`$a, b/a, c/a, y_1, y_2, y_3, z_3$

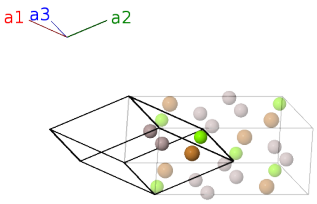
Other compounds with this structure

$CaNiGa_2$, $CeCuPd_2$, $EuIrSn_2$, $EuPdIn_2$, $EuPdSn_2$, $LaPdIn_2$, $NdCuPd_2$, $PPdNi_2$, $PdSrMg_2$, $PrCuPd_2$, $ScNiAl_2$, $SmCuPd_2$, $TaBCo_2$, $YNiAl_2$, $YbAuIn_2$, $YbPdIn_2$

- This is often referred to as an "S-phase precipitate." It can be considered as the ternary version of the Re_3B structure.

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Cu 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)	Cu 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)	Mg I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_7}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	Al I
$\mathbf{B_8}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(8f)	Al I

References

[1] B. Heying, R.-D. Hoffmann, and R. Pöttgen, *Structure Refinement of the S-Phase Precipitate $MgCuAl_2$*, Z. Naturforsc. B **60**, 491–494 (2005).