$CdAl_2S_4$ ($E3$) Structure: A2BC4_tI14_82_bc_a_g-001

This structure originally had the label `A2BC4_tI14_82_bc_a_g`. Calls to that address will be redirected here.

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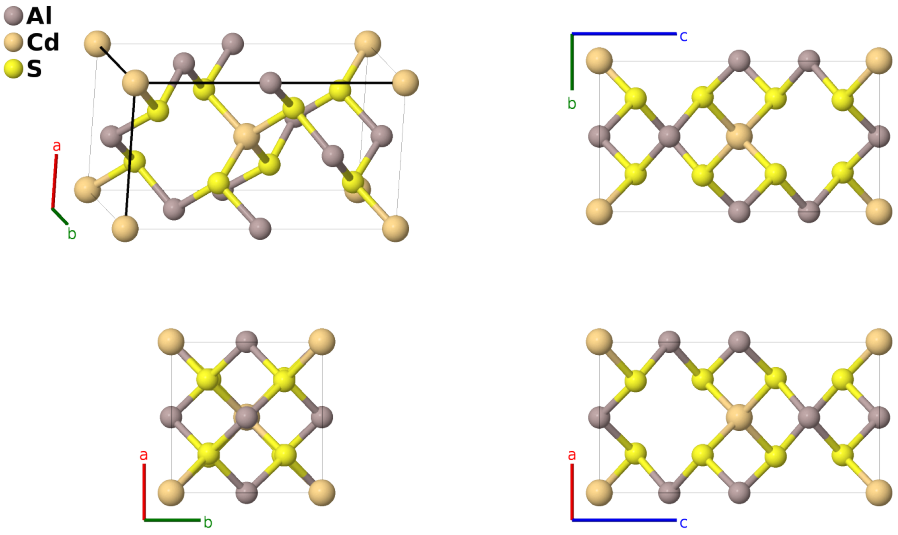
https://aflow.org/p/S1AD

https://aflow.org/p/A2BC4_tI14_82_bc_a_g-001



Prototype	Al_2CdS_4
AFLOW prototype label	A2BC4_tI14_82_bc_a_g-001
***Strukturbericht* designation**	$E3$
ICSD	25634
Pearson symbol	tI14
Space group number	82
Space group symbol	$I\bar{4}$
AFLOW prototype command	`aflow --proto=A2BC4_tI14_82_bc_a_g-001 --params=`$a, c/a, x_4, y_4, z_4$

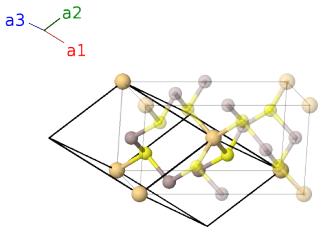
Other compounds with this structure

$CdAl_2Se_4$, $CdAl_2Te_4$, $CdGa_2S_4$, $CdGa_2Se_4$, $CdGa_2Te_4$, $CoGa_2S_4$, $FeGa_2S_4$, $HfGa_2Se_4$, β-$HgAg_2I_4$, $HgAl_2S_4$, $HgAl_2Se_4$, $HgAl_2Te_4$, $HgGa_2S_4$, $HgGa_2Te_4$, $HgIn_2Se_4$, $HgIn_2Te_4$, $ZnGa_2S_4$, $ZnGa_2Se_4$, $ZnGa_2Te_4$, $ZnIn_2Se_4$, $ZnIn_2Te_4$

- When $c = 2a$ and $x = y = 1/4$, and $z = 1/8$ the atoms are on the sites of the diamond (A4) structure, but of course there are defects. Removing the Al-I (2b) atom transforms this to the BPO_4 ($H0_7$) structure.
- (Pearson, 1967) gives this the designation $E3$, without any subscript. It should be defined as $E3_a$, but as he did not put any other structures into this subcategory, we will leave it as is.

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cd I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Al I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(2c)	Al II
$\mathbf{B_4}$	=	$(y_4 + z_4)\,\mathbf{a}_1 + (x_4 + z_4)\,\mathbf{a}_2 + (x_4 + y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_5}$	=	$-(y_4 - z_4)\,\mathbf{a}_1 - (x_4 - z_4)\,\mathbf{a}_2 - (x_4 + y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_6}$	=	$-(x_4 + z_4)\,\mathbf{a}_1 + (y_4 - z_4)\,\mathbf{a}_2 - (x_4 - y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	S I
$\mathbf{B_7}$	=	$(x_4 - z_4)\,\mathbf{a}_1 - (y_4 + z_4)\,\mathbf{a}_2 + (x_4 - y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8g)	S I

References

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[2] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types*, *Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1_3.

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Found in

[1] P. Villars, *$CdAl_2S_4$ Crystal Structure* (2016). PAULING FILE in: Inorganic Solid Phases, SpringerMaterials (online database), Springer, Heidelberg (ed.) SpringerMaterials.