

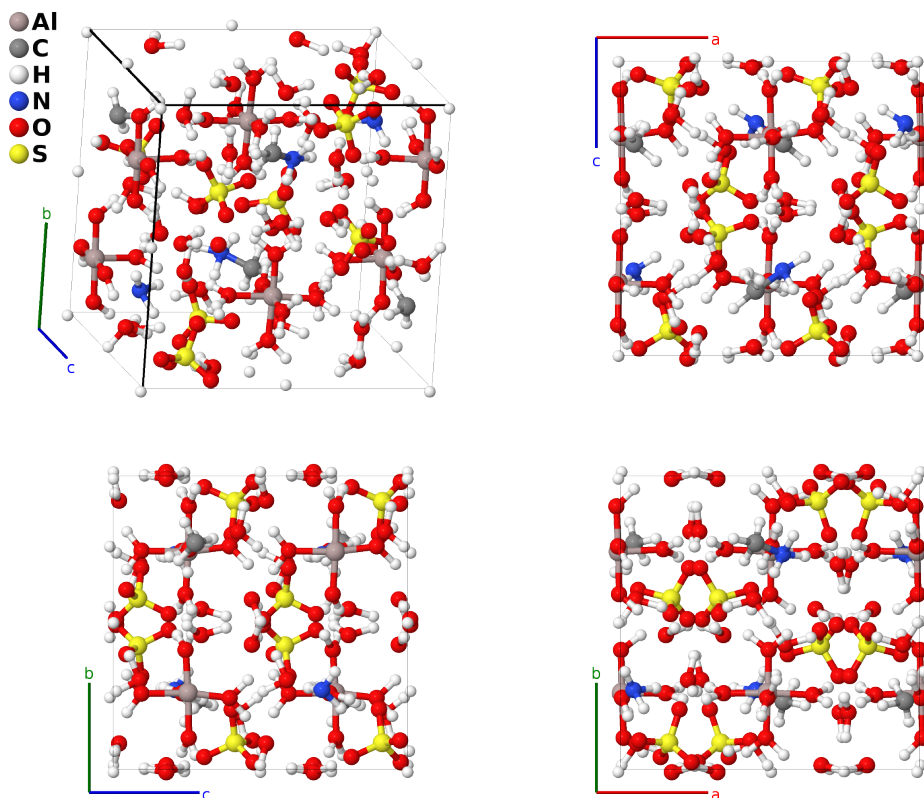
Low Temperature $(\text{NH}_3\text{CH}_3)\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ Structure: ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a-001

This structure originally had the label ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a. Calls to that address will be redirected here.

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<https://aflow.org/p/2B7C>

https://aflow.org/p/ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a-001

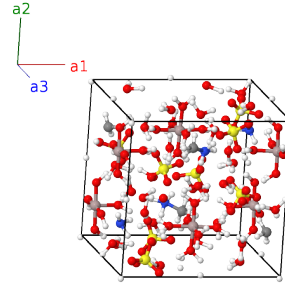


Prototype	$\text{AlCH}_3\text{NO}_2\text{S}_2$
AFLOW prototype label	ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a-001
ICSD	108970
Pearson symbol	oP220
Space group number	29
Space group symbol	$Pca2_1$
AFLOW prototype command	<pre>aflow --proto=ABC30DE20F2_oP220_29_a_a_30a_a_20a_2a-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10, x11, y11, z11, x12, y12, z12, x13, y13, z13, x14, y14, z14, x15, y15, z15, x16, y16, z16, x17, y17, z17, x18, y18, z18, x19, y19, z19, x20, y20, z20, x21, y21, z21, x22, y22, z22, x23, y23, z23, x24, y24, z24, x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29, x30, y30, z30, x31, y31, z31, x32, y32, z32, x33, y33, z33, x34, y34, z34, x35, y35, z35, x36, y36, z36, x37, y37, z37, x38, y38, z38, x39, y39, z39, x40, y40, z40, x41, y41, z41, x42, y42, z42, x43, y43, z43, x44, y44, z44, x45, y45, z45, x46, y46, z46, x47, y47, z47, x48, y48, z48, x49, y49, z49, x50, y50, z50, x51, y51, z51, x52, y52, z52, x53, y53, z53, x54, y54, z54, x55, y55, z55</pre>

- The alums have the general formula $AB(XO_4)_2 \cdot 12H_2O$, where A is a monovalent ion, B is a trivalent ion, and X is a chalcogen. In most cases atom B is aluminum and atom X is sulfur, leading to the name alum.
- All alums have their room-temperature form in space group $Pa\bar{3}$ #205, but the bonding between the A and B ions and the XO_4 complex can be quite different.
- (Lipson, 1935abc) described three general forms of alum based on the sizes of the monovalent ions. Each of these forms was given a *Strukturbericht* designation by (Gottfried, 1937):
 - α -alum, with intermediate sized ions, prototype $KAl(SO_4)_2 \cdot 12H_2O$, $H4_{13}$,
 - β -alum, with large ions, prototype $(NH_3CH_3)Al(SO_4)_2 \cdot 12H_2O$, $H4_{14}$, and
 - γ -alum, with small ions, prototype $NaAl(SO_4)_2 \cdot 12H_2O$, $H4_{15}$.
- This classification scheme is not complete, *e.g.*, (Ledsham, 1968) points out that $NaCr(SO_4)_2 \cdot 12H_2O$ does not fit into any of these categories, and that the actual structure depends on the combination of monovalent and trivalent ions.
- As noted above, the $Pa\bar{3}$ structures of alum are the room temperature form. As the temperature decreases the alum structure may transform. For example, in the temperature range 150-170K the β -alum $(NH_3CH_3)Al(SO_4)_2 \cdot 12H_2O$ transforms into this orthorhombic structure with fully ordered NH_3CH_3 ions.
- The data presented here was taken at 113K.

Simple Orthorhombic primitive vectors

$$\begin{aligned} \mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}} \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Al I
\mathbf{B}_2	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al I
\mathbf{B}_3	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	Al I
\mathbf{B}_4	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	Al I
\mathbf{B}_5	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_6	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_7	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_8	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_9	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_{10}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H I
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	H I

$$\begin{aligned}
\mathbf{B}_{216} &= -\left(x_{54} - \frac{1}{2}\right) \mathbf{a}_1 + y_{54} \mathbf{a}_2 + \left(z_{54} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{54} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{54} \hat{\mathbf{y}} + c \left(z_{54} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{S I} \\
\mathbf{B}_{217} &= x_{55} \mathbf{a}_1 + y_{55} \mathbf{a}_2 + z_{55} \mathbf{a}_3 &= ax_{55} \hat{\mathbf{x}} + by_{55} \hat{\mathbf{y}} + cz_{55} \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{218} &= -x_{55} \mathbf{a}_1 - y_{55} \mathbf{a}_2 + \left(z_{55} + \frac{1}{2}\right) \mathbf{a}_3 &= -ax_{55} \hat{\mathbf{x}} - by_{55} \hat{\mathbf{y}} + c \left(z_{55} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{219} &= \left(x_{55} + \frac{1}{2}\right) \mathbf{a}_1 - y_{55} \mathbf{a}_2 + z_{55} \mathbf{a}_3 &= a \left(x_{55} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{55} \hat{\mathbf{y}} + cz_{55} \hat{\mathbf{z}} & (4a) & \text{S II} \\
\mathbf{B}_{220} &= -\left(x_{55} - \frac{1}{2}\right) \mathbf{a}_1 + y_{55} \mathbf{a}_2 + \left(z_{55} + \frac{1}{2}\right) \mathbf{a}_3 &= -a \left(x_{55} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{55} \hat{\mathbf{y}} + c \left(z_{55} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{S II}
\end{aligned}$$

References

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