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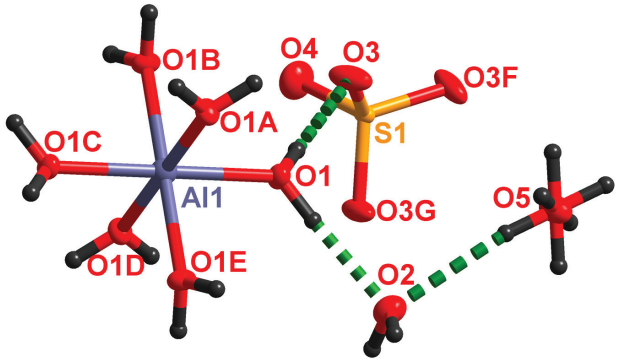
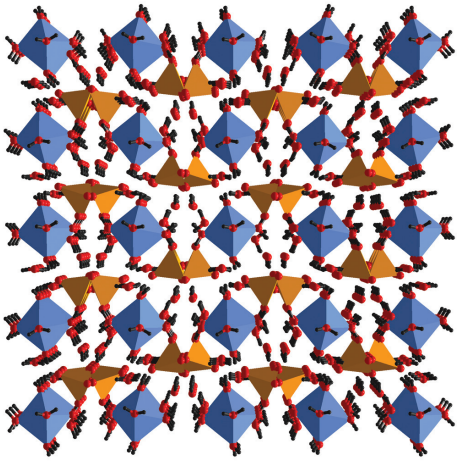
The crystal structure of oxonium hexaquaaluminium disulfate hexahydrate





https://doi.org/10.1515/ncrs-2020-0332
Received July 6, 2020; accepted August 12, 2020; available online October 5, 2020

Abstract

$AlH_{27}S_2O_{21}$, cubic, $Pa\bar{3}$ (no. 205), $a = 12.2403(14)$ Å, $V = 1833.9(6)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0507$, $wR_{ref}(F^2) = 0.1458$, $T = 298$ K.

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CCDC no.: 2022725

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.48 × 0.43 × 0.34 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.44 mm^{-1}
Diffractometer, scan mode:	Bruker D8 Venture,
θ_{max}, completeness:	27.5°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	26703, 706, 0.035
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 676
$N(param)_{refined}$:	51
Programs:	Bruker [1], Olex2 [2], SHELX [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	x	y	z	U_{iso}*/U_{eq}
S1	0.69153(5)	0.19153(5)	0.30847(5)	0.0248(5)
Al1	0.500000	0.500000	0.500000	0.0180(5)
O1	0.51616(15)	0.34834(13)	0.48316(15)	0.0268(6)
H1A	0.568(2)	0.317(3)	0.453(3)	0.040*
H1B	0.465(2)	0.303(2)	0.474(3)	0.040*
O2	0.36262(17)	0.20139(18)	0.45513(19)	0.0402(7)
H2A	0.337(4)	0.208(4)	0.393(2)	0.060*
H2B	0.312(3)	0.207(4)	0.498(3)	0.060*
O3	0.6881(2)	0.2380(3)	0.4183(2)	0.0648(10)
O4	0.7596(2)	0.2596(2)	0.2404(2)	0.0778(16)
O5	0.500000	0.000000	0.500000	0.0574(17)
H5[a]	0.466350	0.060940	0.488040	0.086*

[a]Occupancy: 0.5.

Source of material

This new aluminum sulfate is obtained from the catalyst waste water of automobile exhaust. The exhaust acid of the automobile exhaust catalyst is evaporated to dryness to obtain a yellow solid, and a little water is added to the solid while it is hot to completely dissolve it, and then it is cooled to room temperature to obtain the title compound. Since the impurities in the original solution are so many, it is necessary to recrystallize and purify the crude product. The obtained

crude product is dissolved in a small amount of hot water, and after cooling, pure crystal s of the title compound can be obtained.

Experimental details

SADABS-2016/2 (Bruker, 2016/2) was used for absorption correction. The structure was solved by direct methods and refined using the SHELXL software package [2, 3].

Comment

A variety of structures that are very similar to the structure of the title compound has been reported, such as: $Fe_2(SO_4)_3 \cdot H_2SO_4 \cdot 28H_2O$, $H_3O[Al(SO_4)_2]$, $(H_3O)_2[Al_2(SO_4)_3]_2(SO_4) \cdot 22H_2O$ [4–6]. There are octahedral structures of ML_6 (M is Fe or Al atom, L is a ligand involved in coordination) unit and tetrahedral configuration of sulfate ion.

The upper part of the figure is a structural diagram of the asymmetric unit of the compound mentioned in the title, and there are some hydrogen bonds. The Al1 atom is located in the center of symmetry (0.5, 0.5, 0.5). The O1 atom belonging to the aluminum water complex and the O1A, O1B, O1C, O1D, and O1E atoms obtained through the symmetric operation construct an octahedral shape around the Al1 atom. The O4 atom, O3 atom, and O3F and O3G atoms obtained by the symmetric operation are part of the sulfate anion and the O2 atom belongs to the additional water molecule. O2 and O3 atoms act as electron donors to form hydrogen bonds with hydrogen atoms on O1. The oxonium cation is located at a special position producing a 1/1 disorder, and its hydrogen atom acts as an electron acceptor, forming a hydrogen bond with the O2 atom. $Al(H_2O)_6$ octahedral units, sulfate units, H_3O^+ ions and interstitial water molecules are connected by hydrogen bonds to form the entire crystal structure (lower part of the figure).

Acknowledgements: Our research is supported by 2017 Green Manufacturing System Integration Project of the Ministry of Industry and Information Technology of China and Key Research and Development (R&D) Projects of Shanxi Province of Chnia (201703D321008).

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