

Table 46A-1-001. $\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (GASH). Solubility A [$\text{kg solute}/\text{m}^3 \text{H}_2\text{O}$] in H_2O [56Rez].

T [°C]	A [kg m^{-3}]	T [°C]	A [kg m^{-3}]
22.7	592	75.6	901.45
26.1	637.7	79	940
28.2	686.2	81.7	990.8
42.9	728.9	86	1044
64.45	812.5	88.2	1088.5
70.2	864.2		

Table 46A-1-002. $\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (GASH). Fractional coordinates [$\cdot 10^{-4}$] and temperature parameters [67Sch]. β_{ij} [\AA^2] is defined by Eq. (c) in Introduction.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{12}	β_{23}
N (2)	5595 (5)	3430 (6)	5606 (8)	2.99 (20)	5.59 (28)	3.70 (21)	2.85 (19)	−0.35 (16)	−0.71 (17)
O (5)	8805 (3)	2241 (3)	8005 (6)	1.05 (11)	1.12 (12)	3.91 (16)	0.28 (10)	−0.01 (10)	−0.11 (11)
O (6)	7904 (4)	1161 (4)	2449 (7)	1.63 (13)	1.53 (12)	4.13 (18)	0.60 (11)	0.99 (13)	0.66 (12)
O (9)	5308 (3)	3274 (3)	9437 (6)	1.78 (13)	1.26 (12)	3.01 (15)	0.49 (9)	−0.66 (11)	0.01 (9)
O (10)	5373 (4)	1976 (4)	1773 (7)	2.08 (13)	2.37 (14)	3.37 (16)	1.35 (12)	0.79 (12)	0.95 (13)
S (1)	3486 (1)	0	7607 (5)	1.00 (4)	1.02 (4)	2.16 (5)	0.51	0.04 (4)	0
S (2)	6831 (1)	0	3167 (5)	1.06 (4)	1.14 (4)	2.04 (5)	0.57	0.03 (4)	0
N (1)	1119 (4)	0	5150 (9)	1.56 (18)	1.91 (18)	3.69 (26)	0.95	−0.43 (17)	0
O (1)	4592 (5)	0	8457 (8)	1.52 (14)	1.42 (14)	4.15 (26)	0.71	−1.01 (14)	0
O (2)	5584 (4)	0	2912 (7)	1.54 (14)	1.96 (15)	3.15 (22)	0.98	−0.65 (14)	0
O (3)	3749 (5)	0	6011 (7)	3.49 (20)	3.62 (21)	2.63 (21)	1.81	0.33 (17)	0
O (4)	7073 (4)	0	4756 (7)	2.35 (16)	3.51 (18)	2.65 (19)	1.76	0.14 (14)	0
O (7)	1324 (4)	0	1165 (7)	1.15 (13)	0.84 (15)	2.94 (19)	0.42	−0.66 (13)	0
O (8)	8680 (4)	0	8824 (7)	1.63 (11)	1.75 (11)	2.60 (20)	0.88	−0.69 (12)	0
Al (2)	1/3	2/3	0612 (4)	0.91 (4)	0.91	1.70 (9)	0.46	0	0
C (2)	1/3	2/3	5586 (11)	2.28 (45)	2.28	1.95 (27)	1.14	0	0
C (1)	0	0	5142 (12)	1.12 (21)	1.12	1.88 (35)	0.56	0	0
Al (1)	0	0	0	1.19 (7)	1.19	1.57 (11)	0.60	0	0

Table 46A-1-003. $\text{C}(\text{NH}_2)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ (GASH). Fractional coordinates of hydrogens obtained from different synthesis [67Sch].

	x	y	z
H (1) on N (1)	0.9245	0.1113	0.5092
H (2) on N (2)	0.5729	0.1380	0.5611
H (3) on N (2)	0.7361	0.2309	0.5436
H (4) on O (8)	0.8714	0.0653	0.8611
H (5) on O (7)	0.9287	0.1291	0.1275
H (6) on O (9)	0.7380	0.2061	0.9032
H (7) on O (9)	0.5950	0.1343	0.9000
H (8) on O (10)	0.7957	0.2716	0.2069
H (9) on O (10)	0.8657	0.4078	0.2051

Table 46A-1-004. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH). Interatomic distances [Å] [67Sch].

Al (1)–O (7)	1.871 (6)
Al (1)–O (8)	1.873 (4)
Al (2)–O (9)	1.882 (5)
Al (2)–O (10)	1.872 (6)
C (1)–N (1)	1.313 (3)
C (2)–N (2)	1.319 (7)
S (1)–O (1)	1.505 (6)
S (1)–O (3)	1.462 (8)
S (1)–O (5)	1.477 (3)
S (2)–O (2)	1.481 (5)
S (2)–O (4)	1.451 (7)
S (2)–O (6)	1.463 (5)

Table 46A-1-005. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH). Bond angles [°] [67Sch]. The atom with primed number is related with the one with unprimed number by symmetry operations.

O (7)–Al (1)–O (7')	91.5 (2)
O (7)–Al (1)–O (8)	88.3 (2)
O (8)–Al (1)–O (8')	92.0 (2)
O (9)–Al (2)–O (9')	91.8 (2)
O (9)–Al (2)–O (10)	88.1 (2)
O (10)–Al (2)–O (10')	92.3 (2)
O (1)–S (1)–O (3)	108.2 (4)
O (1)–S (1)–O (5)	108.8 (3)
O (3)–S (1)–O (5)	110.2 (3)
O (5)–S (1)–O (5')	110.7 (3)
O (2)–S (2)–O (4)	110.2 (4)
O (2)–S (2)–O (6)	108.8 (3)
O (4)–S (2)–O (6)	110.7 (3)
O (6)–S (2)–O (6')	108.8 (3)
H (1)–N (1)–H (1')	120 (5)
H (2)–N (2)–H (3)	133 (6)
H (4)–O (8)–H (4')	119 (4)
H (5)–O (7)–H (5')	123 (6)
H (6)–O (9)–H (7)	109 (5)
H (8)–O (10)–H (9)	118 (6)

Table 46A-1-006. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH) family. $c_{\lambda\mu}$ and $s_{\lambda\mu}$ [59Hau1].

Compound	c_{11}	c_{33}	c_{12}	c_{13}	c_{44}	$c_{66} [= \frac{1}{2} (c_{11} - c_{12})]$	c_{14}
	[10 ¹⁰ Pa]						
C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O (GASH)	4.475	1.438	2.835	1.345	0.92	0.820	0.295
C(NH ₂) ₃ Ga(SO ₄) ₂ · 6H ₂ O (GGaSH)	4.378	1.446	2.853	1.413	0.92	0.763	0.305
C(NH ₂) ₃ Al(SeO ₄) ₂ · 6H ₂ O (GASeH)	4.293	1.361	2.688	1.380	0.815	0.803	0.316
C(NH ₂) ₃ Ga(SeO ₄) ₂ · 6H ₂ O (GGaSeH)	4.040	1.353	2.54	1.428	0.81	0.750	0.304
	s_{11}	s_{33}	s_{12}	s_{13}	s_{44}	$s_{66} [= 2 (s_{11} - s_{12})]$	s_{14}
	[10 ⁻¹¹ Pa ⁻¹]						
C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O (GASH)	4.489	10.604	-2.403	-1.951	12.287	13.785	-2.210
C(NH ₂) ₃ Ga(SO ₄) ₂ · 6H ₂ O (GGaSH)	4.896	11.189	-2.658	-2.186	12.530	15.018	-2.504
C(NH ₂) ₃ Al(SeO ₄) ₂ · 6H ₂ O (GASeH)	4.870	12.265	-2.478	-2.425	14.479	14.696	-2.849
C(NH ₂) ₃ Ga(SeO ₄) ₂ · 6H ₂ O (GGaSeH)	5.334	13.64	-2.529	-2.960	14.561	15.726	-2.951

Table 46A-1-007. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH) family. Refractive indices [59Hau1]. $\lambda = 588.9$ nm.

Compound	n_o	n_e
C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O (GASH)	1.5305	1.4416
C(NH ₂) ₃ Ga(SO ₄) ₂ · 6H ₂ O (GGaSH)	1.5374	1.4513
C(NH ₂) ₃ Al(SeO ₄) ₂ · 6H ₂ O (GASeH)	1.5635	1.4713
C(NH ₂) ₃ Ga(SeO ₄) ₂ · 6H ₂ O (GGaSeH)	1.5709	1.4810

Table 46A-1-008. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH) family. e^2qQ/h and $d(e^2qQ/h)/dT$ for ²⁷Al and ⁶⁹Ga [61Bur]. e^2qQ/h : quadrupole coupling constant.

Compound	Site ^{b)}	e^2qQ/h ^{c)} [kHz] 23 °C	$d(e^2qQ/h)/dT$ ^{c)} [kHz · K ⁻¹]
C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O (GASH)	(1)	± 23	0.575
	(2)	∓ 30	0.411
C(NH ₂) ₃ Al(SeO ₄) ₂ · 6H ₂ O (GASeH)	(1)	± 300	0.525
	(2)	± 200	0.228
C(NH ₂) ₃ Ga(SO ₄) ₂ · 6H ₂ O (GGaSH)	(1)	∓ 485(∓ 253) ^{c)}	1.96(102)
	(2)	∓ 635(∓ 331)	1.51(787)
C(NH ₂) ₃ Ga(SeO ₄) ₂ · 6H ₂ O (GGaSeH)	(1)	± 78(± 41)	2.29(119)
	(2)	∓ 197(∓ 103)	1.13(589)
C(ND ₂) ₃ Al(SO ₄) ₂ · 6D ₂ O ^{a)}	(1)	± 23	0.575
	(2)	∓ 30	0.411

^{a)} By comparing the proton resonance in this sample with that obtained in GASH, this compound is 85 % deuterated.

^{b)} Of the three Al or Ga ions per cell, two are equivalent to each other and called site (2). The other one is called site (1).

^{c)} The values of e^2qQ/h and its temperature derivative for ⁷¹Ga are multiplied by 0.521 and given in parentheses in this column.

Table 46A-1-009. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH) family. e^2qQ/h and η of ¹⁴N at $T = 77$ K [73Oja]. e^2qQ/h : quadrupole coupling constant, η : symmetry parameter.

Compound	e^2qQ/h [kHz]	η
C(NH ₂) ₃ Al(SO ₄) ₂ · 6H ₂ O (GASH)	3575.4	0.39475
C(NH ₂) ₃ Cr(SO ₄) ₂ · 6H ₂ O (GCrSH)	3.559.4	0.39866
C(NH ₂) ₃ Al(SeO ₄) ₂ · 6H ₂ O (GASeH)	3556.8	0.40643
C(NH ₂) ₃ Ga(SO ₄) ₂ · 6H ₂ O (GGaSH)	3558.1	0.39918

Table 46A-1-010. C(NH₂)₃Al(SO₄)₂ · 6H₂O (GASH). ESR data of Cr³⁺, Fe³⁺ and Mn²⁺.

Paramagnetic center	Site	<i>S</i>	H	ν	<i>T</i>	<i>g</i> -factor ^{a)} ^{b)}	FS ^{a)} ^{b)}	HFS	Ref.
				[GHz]	[K]		<i>D, a, F</i> [10 ⁻² m ⁻¹]	<i>A</i> [10 ⁻² m ⁻¹]	
Cr ³⁺	Al ³⁺	3/2	(5)	9.3	290	I: 1.980(3)	I: <i>D</i> = 750(2)		57Bog
						II: 1.977(1)	II: <i>D</i> = 590(2)		
					373	I: 1.980(5)	I: <i>D</i> = 610(4)		
						II: 1.980(2)	II: <i>D</i> = 488(4)		
				9	35	1.975(5)	I: <i>D</i> = 1090(50)		58Dan
							II: <i>D</i> = 850(30)		
					77	1.975(5)	I: <i>D</i> = 1050(30)		
							II: <i>D</i> = 822(10)		
					195	1.975(5)	I: <i>D</i> = 882(10)		
							II: <i>D</i> = 696(6)		
Fe ³⁺	Al ³⁺	5/2	(7)	9.6, 23.4	77	I: 2.003	I: <i>D</i> = -1950.6		62Bro
							<i>a</i> = 593.0		
							<i>F</i> = 1639		
						II: 2.003	II: <i>D</i> = -1890.2		
							<i>a</i> = 539.6		
							<i>F</i> = 1520		
					293	I: 2.003	I: <i>D</i> = -1850.8		
							<i>a</i> = 219.7		
							<i>F</i> = 1053		
						II: 2.003	II: <i>D</i> = -1760.1		
Mn ²⁺	Al ³⁺	5/2	(7)	9	RT	2.004	<i>a</i> = 205.9		69Mil
							<i>F</i> = 1005		
							<i>D</i> = 371, 344	-87.5	
							(<i>a</i> - <i>F</i>) ≈ 10		

^{a)} Two sets of spectra, a total of six lines, were observed.^{b)} Spectrum II has twice the intensity of I.