

Table 46A-4-001. C(NH₂)₃Ga(SO₄)₂ · 6H₂O (GGaSH). Fractional coordinates [59Gel].

Atom	Position	x	y	z	
Ga ³⁺ (1)	1a	0	0	0.000	
Ga ³⁺ (2)	2b	$\frac{1}{3}$	$\frac{2}{3}$	0.059	
S (1)	3c	0.351	0	−0.250	
S (2)	3c	−0.318	0	0.306	
O (1)*	3c	0.455	0	−0.156	
O (2)*	3c	−0.433	0	0.238	
O (3)**	3c	0.386	0	−0.409	
O (4)**	3c	−0.328	0	0.470	
O (5***)	6d	0.342	0.120	−0.220	
O (6***)	6d	−0.314	−0.120	0.258	
O (7)	3c	0.140	0	0.130	
O (8)	3c	−0.144	0	−0.135	
O (9)	6d	−0.477	0.333	−0.066	
O (10)	6d	0.476	−0.336	0.174	
C (1)	1a	0	0	0.50	
C (2)	2b	$\frac{1}{3}$	$\frac{2}{3}$	0.52	*) The [SO ₄] “basal” O atoms in the symmetry planes.
N (1)	3c	0.113	0	0.50	**) The [SO ₄] “peak” O atoms in the symmetry planes.
N (2)	6d	0.553	0.333	0.52	***) The [SO ₄] “basal” O atoms related by the symmetry planes.
H (1)	6d	0.198	0.085	0.50	
H (2)	6d	0.553	0.418	0.52	
H (3)	6d	0.469	0.248	0.52	

Table 46A-4-002. C(NH₂)₃Ga(SO₄)₂ · 6H₂O (GGaSH). Interatomic distances [59Gel].

Distances	[Å]	Distances	[Å]
Ga ³⁺ –H ₂ O distances:		H ₂ O–[SO ₄] oxygen distances:	
Ga(1)–O(7)	2.04	O(7)–O(6)	2.54
Ga(1)–O(8)	2.10	O(8)–O(5)	2.61
Ga(2)–O(9)	2.05	O(10)–O(6)	2.63
Ga(2)–O(10)	2.04	O(9)–O(1)	2.51
H ₂ O–H ₂ O distances:		O(10)–O(2)	2.59
O(7)–O(7)	2.87	O(9)–O(5)	2.64
O(8)–O(8)	2.95	N–O distances:	
O(7)–O(8)	2.94	N(1)–O(2)	3.33
O(9)–O(9)	2.94	N(1)–O(4)	3.42
O(10)–O(10)	2.92	N(2)–O(3)	3.33
O(9)–O(10)	2.77	N(2)–O(4)	2.67
		Guanidinium hydrogen–[SO ₄] oxygen distances:	
		H(1)–O(3)	2.98
		H(1)–O(4)	2.50
		H(2)–O(3)	4.35
		H(2)–O(4)	2.36
		H(3)–O(3)	2.67
		H(3)–O(4)	2.34

Table 46A-4-003. C(NH₂)₃Ga(SO₄)₂ · 6H₂O (GGaSH). ESR data of Cr³⁺ solved in GGaSH [61Bur].

Paramagnetic center	Site	<i>S</i>	H	<i>ν</i> [GHz]	<i>T</i> [K]	<i>g</i> -factor	FS ^{a)} <i>D</i> [10 ⁻² m ⁻¹]
Cr ³⁺	Ga ³⁺	3/2	(5)	9	77	1.978	I: <i>D</i> = 866 II: <i>D</i> = 664
					297	1.976	I: <i>D</i> = 576 II: <i>D</i> = 456

^{a)} Spectrum II has twice the intensity of I.