

Table 46A-3-001. C(NH₂)₃Cr(SO₄)₂ · 6H₂O (GCrSH). Fractional coordinates [$\cdot 10^{-4}$] and temperature parameters β_{ij} [\AA^2] [67Sch]. β_{ij} is defined by Eq. (c) in Introduction.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
N (2)	5606 (7)	3431 (7)	5608 (9)	3.59 (27)	5.36 (34)	3.77 (24)	2.73 (24)	−0.41 (23)	0.26 (23)
O (5)	8801 (4)	2251 (4)	7956 (7)	1.03 (15)	1.39 (14)	4.56 (21)	0.36 (14)	0.25 (14)	0.13 (14)
O (6)	7922 (5)	1174 (4)	2522 (7)	2.47 (20)	1.51 (18)	4.19 (20)	0.80 (17)	0.57 (14)	0.58 (15)
O (9)	5239 (5)	3269 (4)	9402 (6)	2.52 (19)	1.82 (18)	3.24 (18)	0.83 (14)	−1.22 (15)	−0.13 (16)
O (10)	5336 (5)	1928 (5)	1821 (7)	2.34 (20)	2.64 (26)	4.18 (22)	1.74 (18)	0.99 (16)	1.24 (17)
S (1)	3498 (2)	0	7560 (4)	1.14 (5)	1.23 (5)	2.38 (6)	0.61	0.00 (5)	0
S (2)	6838 (2)	0	3223 (4)	1.23 (5)	1.25 (5)	2.28 (6)	0.62	−0.02 (5)	0
N (1)	1132 (5)	0	5175 (10)	1.16 (19)	1.79 (21)	4.21 (35)	0.90	0.00 (21)	0
O (1)	4577 (6)	0	8419 (8)	2.06 (22)	1.34 (18)	4.08 (30)	0.67	−1.23 (19)	0
O (2)	5605 (5)	0	2966 (7)	1.79 (30)	2.15 (19)	2.90 (23)	1.08	−0.38 (17)	0
O (3)	3765 (6)	0	5989 (8)	3.28 (24)	3.88 (27)	2.88 (25)	1.94	−0.13 (21)	0
O (4)	7080 (5)	0	4795 (7)	2.78 (20)	3.02 (22)	2.37 (22)	1.51	−0.41 (18)	0
O (7)	1378 (6)	0	1169 (8)	1.76 (19)	1.81 (19)	2.23 (26)	0.91	−0.73 (18)	0
O (8)	8622 (5)	0	8768 (8)	1.88 (19)	2.22 (21)	3.18 (27)	1.11	−1.15 (18)	0
Cr (2)	1/3	2/3	0634 (3)	0.96 (3)	0.96	1.46 (6)	0.48	0	0
C (2)	1/3	2/3	5584 (12)	2.24 (21)	2.24	2.20 (31)	1.12	0	0
C (1)	0	0	5166 (15)	1.40 (28)	1.40	1.84 (43)	0.70	0	0
Cr (1)	0	0	0	1.04 (5)	1.04	1.44 (7)	0.52	0	0

Table 46A-3-002. C(NH₂)₃Cr(SO₄)₂ · 6H₂O (GCrSH). Fractional coordinates of hydrogen atoms from different synthesis [67Sch].

	x	y	z
H (1) on N (1)	0.9202	0.1090	0.5194
H (2) on N (2)	0.5846	0.1407	0.5473
H (3) on N (2)	0.7349	0.2288	0.5602
H (4) on O (8)	0.8626	0.0772	0.8528
H (5) on O (7)	0.9239	0.1263	0.1302
H (6) on O (9)	0.7377	0.2028	0.8949
H (7) on O (9)	0.6066	0.1246	0.9060
H (8) on O (10)	0.8280	0.2958	0.1934
H (9) on O (10)	0.8664	0.4068	0.2095

Table 46A-3-003. C(NH₂)₃Cr(SO₄)₂ · 6H₂O (GCrSH). Interatomic distances [\AA] [67Sch].

Cr (1)–O (7)	1.934 (5)
Cr (1)–O (8)	1.966 (7)
Cr (2)–O (9)	1.983 (6)
Cr (2)–O (10)	1.934 (6)
C (1)–N (1)	1.331 (6)
C (2)–N (2)	1.308 (8)
S (1)–O (1)	1.487 (7)
S (1)–O (3)	1.454 (8)
S (1)–O (5)	1.483 (6)
S (2)–O (2)	1.486 (7)
S (2)–O (4)	1.449 (7)
S (2)–O (6)	1.472 (7)

Table 46A-3-004. C(NH₂)₃Cr(SO₄)₂ · 6H₂O (GCrSH). Bond angles [°] [67Sch]. The atom with primed number is related with the one with unprimed number by symmetry operations.

O (7) – Cr (1) – O (7')	91.3 (3)
O (7) – Cr (1) – O (8)	88.0 (3)
O (8) – Cr (1) – O (8')	93.0 (3)
O (9) – Cr (2) – O (9')	91.6 (2)
O (9) – Cr (2) – O (10)	88.4 (2)
O (10) – Cr (2) – O (10')	92.2 (2)
O (1) – S (1) – O (3)	109.0 (4)
O (1) – S (1) – O (5)	108.2 (3)
O (3) – S (1) – O (5)	110.3 (3)
O (5) – S (1) – O (5')	110.9 (3)
O (2) – S (2) – O (4)	110.4 (4)
O (2) – S (2) – O (6)	108.7 (3)
O (4) – S (2) – O (6)	110.1 (3)
O (6) – S (2) – O (6')	108.5 (4)
H (1) – N (1) – H (1')	125 (6)
H (2) – N (2) – H (3)	124 (6)
H (4) – O (8) – H (4')	115 (5)
H (5) – O (7) – H (5')	133 (6)
H (6) – O (9) – H (7)	104 (5)
H (8) – O (10) – H (9)	104 (6)