Table 45A-6-001. $CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$ (MASD). Crystal structure of phase I [57Oka]. Fractional coordinates and isotropic temperature parameters. *B* is defined by Eq. (e) in Introduction. Wyckoff notations are given in parentheses. See also Fig. 45A-6-004.

		x	*y*	*z*	*B* [Å^2]
4 Al	(a)	0.5000	0.5000	0.0000	1.00
8 S	(c)	0.3329	0.3329	0.3329	1.12
8 $O_{S(1)}$	(c)	0.2639	0.2639	0.2639	3.12
24 $O_{S(2)}$	(d)	0.2808	0.3491	0.4372	2.71
24 O (1)	(d)	0.5029	0.5024	0.1507	1.98
24 O (2)	(d)	0.2288	0.3331	0.0540	2.69
4$CH_3NH_3^+$	(d)	0.4449	0.5264	0.5348	4.44

Table 45A-6-002. $CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$ (MASD). Lattice constants *a*, *b*, *c*, and volume expansion coefficient γ at various temperatures [69Koz].

T	*a*	*b*	*c*	γ
K	Å			10^{-6} K^{-1}
291	12.242	—	—	35
221	12.232	—	—	33
199	12.229	—	—	—
155	12.250	12.214	12.200	−133
130	12.248	12.236	12.220	− 69
115	12.246	12.240	12.230	− 31
78	12.242	—	—	—

Table 45A-6-003. $CH_3NH_3Al(SO_4)_2 \cdot 12H_2O$ (MASD). ESR data [55Bak, 56Bak, 54Ble, 61Bog].

Paramagnetic center	Site	*S*	**H**	ν [GHz]	*T* [K]	*g*-factor	FS *D*, *E*, *a*, *F* [10^{-2} m^{-1}]	Ref.
Cr^{3+}	Al^{3+}	3/2	(5)	9; 3	90	1.975(10)	*D* = 959(20) *E* = 90(10)	55Bak, 56Bak [1])
					20	1.977(3)	*D* = –958(4) *E* = –92(8)	
Fe^{3+}	Al^{3+}	5/2	(7)	9	90		*D* = 1880(140) *a* = 100(40)	54Ble [2])
					90		*D* = +1893(2) *a* ≅ +130 *F* ≅ –40	61Bog [3])

[1]) Zero field splitting δ of the used sample (dilution is 100) is measured directly: $\delta = 1790(30) \cdot 10^{-2}$ m^{-1}; $(2D^2 + E^2)^{1/2} = 1770(20) \cdot 10^{-2}$ m^{-1}.

[2]) Single crystal (dilution is 200).

[3]) Polycrystal (dilution is 100). At 90 K the zero field separation is measured directly; the separation of the $S_z = \pm 3/2$ states from the $\pm 1/2$ is equivalent to 12227(5) MHz, and that of the $\pm 5/2$ from the $\pm 3/2$ to 22043(10) MHz.