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$NH_4Ce(SO_4)_2 \cdot 4H_2O$

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Key indicators: single-crystal X-ray study; T = 298 K; mean σ(S–O) = 0.007 Å; R factor = 0.034; wR factor = 0.068; data-to-parameter ratio = 10.3.

Single crystals of ammonium cerium(III) bis(sulfate) tetrahydrate were grown by slow evaporation of an aqueous sulfate solution containing NH_4^+ and Ce^{3+}. The crystal structure is isotypic with other ammonium rare earth sulfates of the type NH_4*RE*$(SO_4)_2 \cdot 4H_2O$ where complete single-crystal stucture analyses have already been performed for *RE* = La, Sm and Tb. The Ce^{3+} cation is coordinated by nine O atoms, six of which belong to SO_4 groups and three to H_2O molecules. The rare earth cation is in the centre of a distorted tricapped trigonal prism. The structure is held together by moderate hydrogen bonds between the tetrahedral SO_4^{2-} and NH_4^+ groups and the water molecules.

Related literature

The structural arrangement of the title compound is comparable with that of the isotypic compounds NH_4*RE*$(SO_4)_2 \cdot 4H_2O$ with *RE* = Sm (Eriksson *et al.*, 1974), La and Tb (Kepert *et al.*, 1999). Similar coordination polyhedra around the rare earth metal cation are observed for $TlLa(SO_4)_2 \cdot 2H_2O$ (Kaučič *et al.*, 1985), $(NH_4)_8Ce_2(SO_4)_8 \cdot 4H_2O$ (Shan & Huang, 1998), $NaCe(SO_4)_2 \cdot H_2O$ (Blackburn & Gerkin, 1995), $AgCe(SO_4)_2 \cdot H_2O$ (Audebrand *et al.*, 1998) and $NaLa(SO_4)_2 \cdot H_2O$ (Blackburn & Gerkin, 1994).

For related literature, see: Kepert *et al.* (1999).

Experimental

Crystal data

$NH_4Ce(SO_4)_2 \cdot 4H_2O$
M_r = 422.35
Monoclinic, $P2_1/c$
a = 6.673 (2) Å
b = 18.9920 (5) Å
c = 8.808 (2) Å
β = 97.29 (3)°
V = 1107.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.55 mm^{-1}
T = 298 K
0.10 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*MULABS* in *PLATON*; Spek, 2003)
T_{min} = 0.667, T_{max} = 0.772
6836 measured reflections
3225 independent reflections
1489 reflections with $I > 3\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.068
S = 1.05
1489 reflections
145 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −2.62 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ce1—O8^{i}	2.450 (5)	S1—O3^{ii}	1.456 (7)
Ce1—O2	2.545 (6)	S1—O1	1.459 (6)
Ce1—O3	2.420 (7)	S1—O2	1.491 (6)
Ce1—O4	2.578 (6)	S1—O4	1.464 (6)
Ce1—O5	2.530 (6)	S2—O5	1.495 (6)
Ce1—O7	2.573 (6)	S2—O6	1.432 (8)
Ce1—O9	2.523 (6)	S2—O7	1.479 (8)
Ce1—O10	2.554 (6)	S2—O8	1.449 (6)
Ce1—O11	2.482 (7)		

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O12	0.793 (9)	2.167 (10)	2.918 (14)	153.1 (7)
N1—H3$\cdots$O4	0.823 (9)	2.088 (6)	2.882 (12)	165.6 (7)
N1—H4$\cdots$O2^{i}	1.003 (10)	2.157 (6)	3.067 (11)	150.0 (6)
O9—H5$\cdots$O7	0.992 (7)	2.068 (7)	2.998 (10)	156.2 (5)
O9—H6$\cdots$O1^{ii}	0.845 (7)	2.052 (6)	2.738 (9)	138.7 (6)
O11—H9$\cdots$O12^{iii}	0.815 (7)	1.969 (9)	2.776 (11)	174.6 (6)
O11—H10$\cdots$O7^{iv}	0.824 (6)	1.906 (7)	2.705 (9)	176.1 (6)

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $-x+2, -y+1, -z+2$; (iv) $-x+1, -y+1, -z+2$.

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *CRYSTALS*.

The authors thank Marc Leblanc for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2108).

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doi:10.1107/S1600536807024555

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supplementary materials

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$NH_4Ce(SO_4)_2·4H_2O$

M. Boujelben, M. Toumi and T. Mhiri

Comment

Compounds of the type $MCe(SO_4)_2·4H_2O$ (*M* = K, Na, Ag) have already been prepared and characterized by X-ray powder diffraction methods. Although space group and cell parameters were determined (Shan *et al.*, 1998; Blackburn *et al.*, 1995; Blackburn *et al.*, 1994, Kepert *et al.*, 1999), more detailed structural data were not provided. Our particular interest concerned the structure determination and hydrogen bonding of $NH_4Ce^{III}(SO_4)_2·4H_2O$.

The structural arrangement of the title compound (Fig. 1) is very similar to that of the isotypic structures of $NH_4RE(SO_4)_2·4H_2O$ with RE = Sm (Eriksson *et al.*, 1974), La and Tb (Cameron *et al.*, 1999). The Ce^{3+} cation coordinates to nine O atoms, six of which belong to SO_4 groups and three to H_2O molecules. The coordination polyhedron is a distorted tricapped trigonal prism, with O10, O11 and O5 as the top face, O9, O4 and O2 as bottom face and O3, O7 and O8 as capping atoms. A similar coordination of rare earth cations has been observed for $TlLa(SO_4)_2·2H_2O$ (Kaučič *et al.*, 1985), and for $(NH_4)_8Ce_2(SO_4)_8·4H_2O$ (Shan & Huang, 1998). In the La compound, the rare earth cation coordinates to seven O atoms belonging to sulfate groups and to O atoms of two water molecules, whereas in the Ce compound the coordination sphere of the Ce cation solely consists of sulfate O atoms. In $NaCe(SO_4)_2·H_2O$ (Blackburn *et al.*, 1995), $AgCe(SO_4)_2·H_2O$ (Audebrand *et al.*, 1998) and $NaLa(SO_4)_2·H_2O$ (Blackburn *et al.*, 1994) only one water O atom is involved in the oxygen coordination sphere of the rare earth cations.

In the title compound the Ce—O bond lengths range from 2.420 (7) to 2.578 (6) Å [average 2.517 (4) Å; Table 1] and are comparable with those found in $NaCe(SO_4)_2·H_2O$. For $(NH_4)_8Ce_2(SO_4)_8·4H_2O$, shorter Ce—O distances are observed that range from 2.325 (2) to 2.478 (2) Å [average 2.395 (6) Å], caused by the higher oxidation state of Ce^{4+} in this compound and thus a smaller ionic radius. The S—O bond distances in the SO_4 tetrahedron are in the usual range with an average of 1.467 Å for S1 and of 1.463 Å for S2 (Table 1).

The water molecules, NH_4^+ cations and SO_4^{2-} anions are interconnected *via* hydrogen bonds of medium strength, with donator acceptor distances in the range 2.705 (9) to 3.067 (11) Å (Table 2).

Experimental

Aqueous solutions of $Ce(SO_4)_2·4H_2O$, NH_4CN and NH_4Cl were mixed in the molar ratio 1:0.5:0.5 which resulted in a white precipitate. After filtration, the remaining solution was allowed to evaporate. Within a few days small transparent prismatic crystals of $NH_4Ce(SO_4)_2·4H_2O$ were obtained, indicating the reduction of Ce^{4+} to Ce^{3+}.

Refinement

All H atoms were found in difference Fourier maps and were refined freely. The highest peak is located 0.52 Å from O11 and the deepest hole 0.30 Å from H10.

Figures

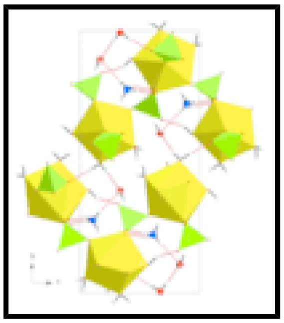

Fig. 1. Projection of the structure along [100]. $[Ce(H_2O)_3O_6]$ polyhedra are yellow, SO_4 tetrahedra are green, O, N and H atoms are displayed as red, blue and white spheres. Hydrogen bonds are indicated with dashed lines.

ammonium cerium(III) bis(sulfate) tetrahydrate

Crystal data

$NH_4Ce(SO_4)_2 \cdot 4H_2O$

$M_r = 422.35$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 6.673$ (2) Å

$b = 18.9920$ (5) Å

$c = 8.808$ (2) Å

$\beta = 97.29$ (3)°

$V = 1107.3$ (4) Å^3

$Z = 4$

$F_{000} = 820$

$D_x = 2.533$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 6883 reflections

$\theta = 1.8$–25.8°

$\mu = 4.55$ mm^{-1}

$T = 298$ K

Prism, transparent

0.10 × 0.08 × 0.06 mm

Data collection

Nonius Kappa CCD area-detector diffractometer

Monochromator: graphite

$T = 298$ K

φ rotation scans with 2° steps

Absorption correction: multi-scan (MULABS in PLATON; Spek, 1998)

$T_{min} = 0.667$, $T_{max} = 0.772$

6836 measured reflections

3225 independent reflections

1489 reflections with $I > 3\sigma(I)$

$R_{int} = 0.042$

$\theta_{max} = 30.0$°

$\theta_{min} = 2.2$°

$h = -9 \rightarrow 9$

$k = -26 \rightarrow 26$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.068$

$S = 1.05$

1489 reflections

145 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

All H-atom parameters refined

Method, part 1, Chebychev polynomial, (Watkin, 1994; *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)]
where A_i are the Chebychev coefficients listed belo*w* and x = *F* /*F*max Method = robust *w*eighting (*P*rince, 1982) W = [*w*eight] * $[1-(\text{delta}F/6*\text{sigma}F)^2]^2$ A_i are: 0.119E + 04 -0.128E + 04 956.
*P*rince, E. (1982). Mathematical Techniques in Crystallography and Materials Science. Ne*w* York: Springer-Verlag.
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$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.00$ e Å^{-3}

$\Delta\rho_{\min} = -2.62$ e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Ce1	0.64763 (5)	0.37838 (2)	0.78484 (4)	0.0152
S1	0.6215 (3)	0.22283 (10)	0.9125 (2)	0.0227
S2	0.1859 (2)	0.42436 (10)	0.7628 (3)	0.0268
O1	0.5880 (11)	0.1595 (3)	0.8189 (7)	0.0339
O2	0.4532 (9)	0.2738 (3)	0.8726 (8)	0.0299
O3	0.6324 (14)	0.2963 (4)	0.5734 (8)	0.0477
O4	0.8046 (9)	0.2604 (3)	0.8841 (8)	0.0317
O5	0.2958 (9)	0.3919 (4)	0.6427 (7)	0.0421
O6	0.1221 (12)	0.4953 (4)	0.7296 (18)	0.0859
O7	0.3358 (10)	0.4220 (5)	0.9017 (9)	0.0481
O8	0.0153 (8)	0.3808 (4)	0.7888 (9)	0.0384
O9	0.7475 (12)	0.3922 (4)	1.0692 (7)	0.0424
O10	0.6715 (11)	0.4456 (4)	0.5367 (8)	0.0374
O11	0.6946 (14)	0.5064 (4)	0.8336 (8)	0.0433
N1	1.1550 (14)	0.2781 (5)	1.1103 (10)	0.0465
O12	1.1383 (12)	0.3893 (5)	1.3333 (11)	0.0566
H1	1.1104	0.3072	1.1611	0.0500*
H2	1.1757	0.2387	1.1504	0.0500*
H3	1.0699	0.2738	1.0347	0.0500*
H4	1.2787	0.2884	1.0602	0.0500*
H7	0.7780	0.4503	0.4859	0.0500*
H5	0.6188	0.3895	0.9994	0.0500*

H6	0.7483	0.3625	1.1406	0.0500*
H8	0.5980	0.4851	0.5266	0.0500*
H9	0.7458	0.5349	0.7810	0.0500*
H10	0.6884	0.5296	0.9120	0.0500*
H11	1.2719	0.3790	1.3297	0.0500*
H12	1.0854	0.3554	1.3679	0.0500*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.01392 (14)	0.01666 (15)	0.01504 (14)	−0.0010 (2)	0.00201 (8)	−0.0016 (2)
S1	0.0303 (8)	0.0188 (8)	0.0188 (7)	−0.0041 (6)	0.0027 (6)	0.0023 (6)
S2	0.0159 (7)	0.0214 (8)	0.0439 (11)	0.0001 (6)	0.0071 (7)	0.0021 (8)
O1	0.051 (4)	0.028 (3)	0.023 (3)	−0.007 (3)	0.005 (2)	−0.001 (2)
O2	0.026 (2)	0.028 (3)	0.037 (3)	−0.005 (2)	0.010 (2)	0.004 (2)
O3	0.096 (6)	0.022 (3)	0.024 (3)	0.003 (4)	0.004 (4)	−0.008 (3)
O4	0.027 (3)	0.024 (3)	0.042 (4)	−0.001 (2)	0.000 (2)	0.009 (2)
O5	0.022 (2)	0.081 (6)	0.023 (3)	0.021 (3)	0.000 (2)	0.006 (3)
O6	0.033 (4)	0.027 (4)	0.199 (14)	0.011 (3)	0.019 (5)	0.034 (5)
O7	0.028 (3)	0.071 (5)	0.047 (4)	0.002 (3)	0.009 (3)	−0.036 (4)
O8	0.017 (2)	0.035 (3)	0.064 (4)	−0.011 (3)	0.008 (2)	0.008 (4)
O9	0.054 (4)	0.050 (5)	0.021 (3)	−0.016 (3)	−0.005 (2)	0.005 (3)
O10	0.047 (4)	0.036 (3)	0.030 (3)	−0.008 (3)	0.009 (3)	0.012 (3)
O11	0.076 (5)	0.028 (3)	0.031 (3)	−0.009 (3)	0.023 (3)	−0.010 (2)
N1	0.044 (4)	0.053 (5)	0.038 (4)	0.020 (4)	−0.011 (3)	0.003 (4)
O12	0.042 (4)	0.069 (6)	0.055 (4)	0.005 (4)	−0.009 (3)	0.022 (4)

Geometric parameters (Å, °)

Ce1—O8^{i}	2.450 (5)	S2—O6	1.432 (8)
Ce1—S1	3.1736 (18)	S2—O7	1.479 (8)
Ce1—O2	2.545 (6)	S2—O8	1.449 (6)
Ce1—O3	2.420 (7)	O9—H5	0.992
Ce1—O4	2.578 (6)	O9—H6	0.845
Ce1—O5	2.530 (6)	O10—H7	0.891
Ce1—O7	2.573 (6)	O10—H8	0.893
Ce1—O9	2.523 (6)	O11—H9	0.815
Ce1—O10	2.554 (6)	O11—H10	0.824
Ce1—O11	2.482 (7)	N1—H1	0.793
Ce1—H5	1.935	N1—H2	0.831
S1—O3^{ii}	1.456 (7)	N1—H3	0.823
S1—O1	1.459 (6)	N1—H4	1.003
S1—O2	1.491 (6)	O12—H11	0.917
S1—O4	1.464 (6)	O12—H12	0.812
S2—O5	1.495 (6)		
O8^{i}—Ce1—S1	96.44 (18)	O9—Ce1—O10	139.5 (2)
O8^{i}—Ce1—O2	123.9 (2)	O5—Ce1—O11	94.3 (3)
S1—Ce1—O2	27.51 (14)	O7—Ce1—O11	72.9 (3)

O8^{i}—Ce1—O3	88.1 (3)	O9—Ce1—O11	73.4 (2)
S1—Ce1—O3	70.99 (17)	O10—Ce1—O11	68.8 (2)
O2—Ce1—O3	76.0 (2)	O5—Ce1—H5	105.736
O8^{i}—Ce1—O4	69.4 (2)	O7—Ce1—H5	52.304
S1—Ce1—O4	27.05 (13)	O9—Ce1—H5	20.850
O2—Ce1—O4	54.6 (2)	O10—Ce1—H5	143.699
O3—Ce1—O4	71.1 (2)	O11—Ce1—H5	75.529
O8^{i}—Ce1—O5	150.5 (2)	Ce1—S1—O3^{ii}	125.4 (3)
S1—Ce1—O5	100.40 (19)	Ce1—S1—O1	125.3 (3)
O2—Ce1—O5	75.7 (2)	O3^{ii}—S1—O1	109.2 (4)
O3—Ce1—O5	74.9 (3)	Ce1—S1—O2	52.1 (2)
O4—Ce1—O5	124.6 (2)	O3^{ii}—S1—O2	109.6 (4)
O8^{i}—Ce1—O7	148.0 (2)	O1—S1—O2	110.2 (4)
S1—Ce1—O7	94.3 (2)	Ce1—S1—O4	53.2 (2)
O2—Ce1—O7	70.2 (3)	O3^{ii}—S1—O4	110.4 (5)
O3—Ce1—O7	123.9 (3)	O1—S1—O4	112.1 (4)
O4—Ce1—O7	117.3 (3)	O2—S1—O4	105.2 (3)
O8^{i}—Ce1—O9	81.1 (3)	O5—S2—O6	113.8 (7)
S1—Ce1—O9	76.39 (17)	O5—S2—O7	103.4 (3)
O2—Ce1—O9	82.0 (2)	O6—S2—O7	110.5 (7)
O3—Ce1—O9	144.2 (2)	O5—S2—O8	110.0 (5)
O4—Ce1—O9	73.1 (2)	O6—S2—O8	110.5 (5)
O8^{i}—Ce1—O10	80.3 (2)	O7—S2—O8	108.3 (5)
S1—Ce1—O10	141.35 (17)	Ce1—O2—S1	100.4 (3)
O2—Ce1—O10	137.7 (2)	Ce1—O3—S1^{iii}	154.4 (5)
O3—Ce1—O10	70.4 (2)	Ce1—O4—S1	99.8 (3)
O4—Ce1—O10	131.1 (2)	Ce1—O5—S2	101.5 (3)
O8^{i}—Ce1—O11	82.8 (3)	Ce1—O7—S2	100.1 (3)
S1—Ce1—O11	149.54 (17)	Ce1^{iv}—O8—S2	144.5 (5)
O2—Ce1—O11	140.3 (2)	H5—O9—H6	110.455
O3—Ce1—O11	139.1 (2)	Ce1—O10—H7	128.308
O4—Ce1—O11	139.1 (3)	Ce1—O10—H8	114.254
O8^{i}—Ce1—H5	101.977	H7—O10—H8	109.248
S1—Ce1—H5	74.861	H9—O11—H10	101.042
O2—Ce1—H5	70.786	H1—N1—H2	116.347
O3—Ce1—H5	145.265	H1—N1—H3	104.775
O4—Ce1—H5	81.389	H2—N1—H3	108.423
O5—Ce1—O7	54.4 (2)	H1—N1—H4	119.964
O5—Ce1—O9	126.3 (2)	H2—N1—H4	105.124
O7—Ce1—O9	72.2 (3)	H3—N1—H4	100.646
O5—Ce1—O10	71.4 (2)	H11—O12—H12	108.302
O7—Ce1—O10	108.8 (3)		

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y+1/2, z+1/2$; (iii) $x, -y+1/2, z-1/2$; (iv) $x-1, y, z$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O12	0.793 (9)	2.167 (10)	2.918 (14)	153.1 (7)
N1—H3···O4	0.823 (9)	2.088 (6)	2.882 (12)	165.6 (7)
N1—H4···O2^{i}	1.003 (10)	2.157 (6)	3.067 (11)	150.0 (6)
O9—H5···O7	0.992 (7)	2.068 (7)	2.998 (10)	156.2 (5)
O9—H6···O1^{ii}	0.845 (7)	2.052 (6)	2.738 (9)	138.7 (6)
O11—H9···O12^{v}	0.815 (7)	1.969 (9)	2.776 (11)	174.6 (6)
O11—H10···O7^{vi}	0.824 (6)	1.906 (7)	2.705 (9)	176.1 (6)

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, −*y*+1/2, *z*+1/2; (v) −*x*+2, −*y*+1, −*z*+2; (vi) −*x*+1, −*y*+1, −*z*+2.

Fig. 1