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Redetermination of dicerium(III) tris(sulfate) tetrahydrate

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Ce–O) = 0.003 Å; R factor = 0.027; wR factor = 0.067; data-to-parameter ratio = 10.2.

$Ce_2(SO_4)_3(H_2O)_4$ was obtained hydrothermally from an aqueous solution of cerium(III) oxide, trimethylamine and sulfuric acid. The precision of the structure determination has been significantly improved compared with the previous result [Dereigne (1972). *Bull. Soc. Fr. Mineral. Cristallogr.* **95**, 269–280]. The coordination about the two Ce atoms is achieved by seven and six bridging O atoms from sulfate anions. Each S atom makes four S—O—Ce linkages through bridging O atoms. The coordination sphere of each Ce is completed by two water molecules, which act as terminal ligands.

Related literature

For related literature, see: Doran *et al.* (2002); Li *et al.* (1998); Plévert *et al.* (2001); Shi (1987); Xu, Cheng & You (2006); Xu, Ding *et al.* (2006); Yuan *et al.* (2004); Zhang *et al.* (2004). For the previous structure determination, see: Dereigne (1972).

Experimental

Crystal data

$Ce_2(SO_4)_3(H_2O)_4$
M_r = 640.48
Monoclinic, $P2_1/n$
a = 13.1257 (14) Å
b = 7.2520 (8) Å
c = 13.3823 (14) Å
β = 92.5720 (10)°
V = 1272.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.65 mm^{-1}
T = 293 (2) K
0.13 × 0.12 × 0.10 mm

Data collection

Bruker APEX2 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.437, T_{max} = 0.515
(expected range = 0.394–0.466)
5923 measured reflections
2201 independent reflections
2071 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.067
S = 1.09
2201 reflections
215 parameters
16 restraints
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −2.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ce1—O10	2.449 (2)	Ce2—O1^{iii}	2.354 (3)
Ce1—O7	2.465 (3)	Ce2—O4^{iv}	2.430 (3)
Ce1—O12^{i}	2.476 (4)	Ce2—O5^{iii}	2.470 (3)
Ce1—O11^{ii}	2.517 (3)	Ce2—O6^{v}	2.489 (3)
Ce1—O4*W*	2.524 (3)	Ce2—O3*W*	2.494 (3)
Ce1—O3	2.547 (3)	Ce2—O2*W*	2.497 (3)
Ce1—O3^{i}	2.621 (3)	Ce2—O9	2.529 (4)
Ce1—O1*W*	2.647 (3)	Ce2—O8	2.659 (3)
Ce1—O11	2.710 (3)		
O10—Ce1—O3	150.11 (9)	O3—Ce1—O11	53.24 (9)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2049).

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supplementary materials

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X. Xu

Comment

Over the past decades, the design and synthesis of new three–dimensional solid state materials have received great attention, due to their functional applications in catalysis and optical device. As the building elements germanium has been choosen to synthesize new porous materials (Li *et al.*, 1998; Plévert *et al.*, 2001; Xu, Cheng & You, 2006; Xu, Ding *et al.*, 2006). In the last few years, an important advance in three dimensional inorganic materials has been achieved by study of lanthanide sulfates frameworks (Zhang *et al.*,2004; Yuan *et al.*, 2004; Xu, Ding *et al.*, 2006; Doran *et al.*, 2002). In this work, we synthesized the title compound, Cerium(3+) sulfate tetrahydrate, which features a three–dimensional framework. The structure of title compound had been reported previously (Dereigne *et al.*, 1972), however, the precision of redetermination is much improved.

As isostructure with $La_2(SO_4)_3(H_2O)_4$ and $Nd_2(SO_4)_3(H_2O)_4$ (Shi, 1987), the framework of title compound is constructed from CeO_9 and CeO_8 polyhedra and SO_4 tetrahedra. As shown in Fig. 1 and 2, the asymmetric unit contains two Ce^{3+}, three SO_4^{2-} groups and four water molecules, all of which belong to the inorganic framework. The coordination about Ce1 and Ce2, respectively, is achieved by bridging oxygen atoms from sulfate anions. Each S atom makes four S–O–Ce linkages through bridging O atoms. The coordination sphere of each Ce is completed by two water molecules, which act as terminal ligands of Ce^3+^.

The Ce atom has the typical geometrical parameters, with Ce—O distances of 2.354 (3)– 2.710 (3)Å (Table 1). The O—Ce—O angles are between 59.28 (14) and 139.03 (14)°. These bond distances and bond angles are in agreement with those found in similar rare-earth compounds (Zhang *et al.*,2004; Yuan *et al.*, 2004). The geometry of the sulfate ions is unexceptional. Fig. 3 shows the three-dimensional arrangement in the unit cell, displaying the way the different CeO_9 polyhydra are connected by bridging sulfates.

Experimental

Colorless block-shaped crystals were synthesized hydrothermally from a mixture of $CeCl_3{\cdot}6H_2O$, H_2SO_4 (98%), H_2O and trimethylamine(25%). All the chemicals are purchased from Shanghai Chemical Reagent Factory. In a typical synthesis, $CeCl_3{\cdot}6H_2O$(0.2993 g) was dissolved in a mixture of trimethylamine (25%, 0.7893 g) and of water (1 ml) followed by the addition of H_2SO_4 (98%) (0.3528 g) with constant stirring. Finally, the mixture was kept in a 25 ml Teflon-lined steel autoclave at 180 °C for 6 days. The autoclave was slowly cooled to room temperature, and then the product was filtered, washed with distilled water, and dried at room temperature. Colorless block-shaped crystals of the title compound were obtained.

Refinement

The highest peak in the difference map is 1.12 e/Å^3, and 1.26 (2) Å from Ce_2, while the minimum peak is −2.16 (2) Å from Ce_1. 5. The H atoms of water were located from different map, and the O—H distances are restrained to 0.85 (2) Å.

Figures

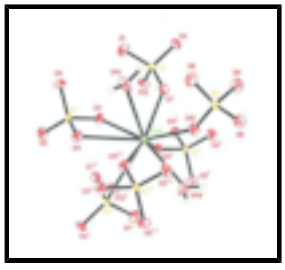

Fig. 1. The coordination of Ce1 for title compound. Displacement ellipsoids at the 70% probability level. Symmetry codes as in Table 1.

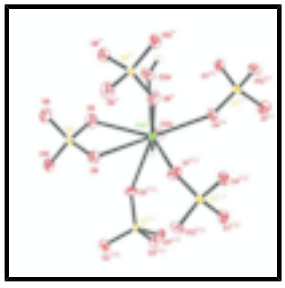

Fig. 2. The coordination of Ce2 for title compound. Displacement ellipsoids at the 70% probability level. Symmetry codes as in Table 1.

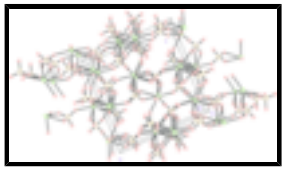

Fig. 3. The crystal packing in the unit cell of $Ce(SO_4)(OH)$.

dicerium(III) tris(sulfate) tetrahydrate

Crystal data

$Ce_2(SO_4)_3(H_2O)_4$	F_{000} = 1200
M_r = 640.48	D_x = 3.343 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2201 reflections
a = 13.1257 (14) Å	θ = 2.1–25.0º
b = 7.2520 (8) Å	μ = 7.65 mm^{-1}
c = 13.3823 (14) Å	T = 293 (2) K
β = 92.5720 (10)º	Block, colourless
V = 1272.5 (2) Å^3	0.13 × 0.12 × 0.10 mm
Z = 4	

Data collection

Bruker APEX2 CCD diffractometer	2201 independent reflections
Radiation source: fine-focus sealed tube	2071 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 293(2)$ K	$\theta_{max} = 25.0^o$
ω scans	$\theta_{min} = 2.1^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$h = -12 \rightarrow 15$
$T_{min} = 0.437$, $T_{max} = 0.515$	$k = -8 \rightarrow 8$
5923 measured reflections	$l = -15 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.027$	Only H-atom coordinates refined
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 1.0649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
2201 reflections	$\Delta\rho_{max} = 1.12$ e Å^{-3}
215 parameters	$\Delta\rho_{min} = -2.16$ e Å^{-3}
16 restraints	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0953 (15)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ce1	0.413692 (17)	0.24066 (3)	0.964316 (18)	0.00669 (14)
Ce2	−0.073660 (17)	0.26197 (3)	0.849355 (18)	0.00793 (14)
S1	0.59971 (8)	0.26189 (10)	1.13380 (8)	0.0068 (2)

S2	0.13846 (6)	0.38957 (12)	0.95722 (7)	0.0088 (2)
S3	0.34712 (6)	−0.10740 (12)	1.15208 (7)	0.0077 (2)
O1	0.3887 (2)	−0.0086 (4)	1.2394 (2)	0.0179 (6)
O2	0.7082 (2)	0.2370 (3)	1.1325 (3)	0.0164 (7)
O3	0.54510 (19)	0.0990 (3)	1.0873 (2)	0.0109 (6)
O4	0.2552 (2)	−0.2061 (4)	1.1792 (2)	0.0153 (6)
O5	0.5660 (2)	0.2917 (4)	1.2352 (2)	0.0152 (6)
O6	0.15247 (19)	0.4888 (4)	1.0522 (2)	0.0174 (6)
O7	0.32350 (19)	0.0207 (4)	1.0695 (2)	0.0137 (6)
O8	0.07908 (19)	0.4978 (4)	0.8833 (2)	0.0134 (6)
O9	0.0762 (3)	0.2206 (4)	0.9727 (3)	0.0158 (7)
O10	0.23802 (19)	0.3357 (4)	0.9218 (2)	0.0163 (6)
O11	0.5637 (2)	0.4210 (4)	1.0702 (2)	0.0121 (6)
O12	0.4231 (3)	−0.2449 (3)	1.1215 (3)	0.0134 (7)
O1W	0.3582 (2)	0.3879 (4)	1.1345 (2)	0.0181 (6)
H1WB	0.2964 (19)	0.371 (5)	1.152 (4)	0.027*
H1WA	0.381 (3)	0.497 (4)	1.138 (4)	0.027*
O2W	−0.13163 (19)	0.1354 (4)	1.0108 (2)	0.0155 (6)
H2WB	−0.185 (2)	0.179 (5)	1.037 (3)	0.023*
H2WA	−0.114 (3)	0.028 (4)	1.030 (3)	0.023*
O3W	−0.0481 (2)	−0.0777 (4)	0.8356 (2)	0.0218 (6)
H3WB	−0.049 (3)	−0.142 (4)	0.889 (2)	0.033*
H3WA	−0.005 (3)	−0.115 (4)	0.793 (3)	0.033*
O4W	0.3708 (3)	0.2180 (5)	0.7790 (3)	0.0245 (8)
H4WB	0.401 (3)	0.147 (6)	0.738 (3)	0.037*
H4WA	0.312 (2)	0.258 (6)	0.758 (4)	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce1	0.0052 (2)	0.00827 (18)	0.0066 (2)	0.00028 (6)	−0.00017 (12)	0.00084 (7)
Ce2	0.0056 (2)	0.00981 (18)	0.0083 (2)	0.00046 (6)	0.00028 (13)	0.00215 (7)
S1	0.0057 (5)	0.0090 (5)	0.0055 (5)	0.0001 (3)	−0.0013 (4)	0.0004 (3)
S2	0.0057 (4)	0.0099 (4)	0.0106 (5)	0.0002 (3)	−0.0002 (3)	−0.0003 (3)
S3	0.0062 (4)	0.0089 (4)	0.0082 (5)	−0.0012 (3)	0.0006 (3)	−0.0009 (3)
O1	0.0210 (14)	0.0193 (14)	0.0134 (14)	−0.0032 (12)	−0.0009 (11)	−0.0063 (12)
O2	0.0081 (16)	0.0242 (17)	0.0169 (18)	0.0004 (10)	0.0000 (13)	−0.0027 (10)
O3	0.0113 (13)	0.0083 (13)	0.0129 (14)	−0.0018 (10)	−0.0022 (11)	0.0008 (11)
O4	0.0084 (14)	0.0212 (13)	0.0164 (15)	−0.0026 (12)	0.0005 (11)	0.0046 (13)
O5	0.0160 (16)	0.0219 (13)	0.0081 (15)	−0.0015 (12)	0.0039 (12)	−0.0029 (13)
O6	0.0148 (14)	0.0217 (14)	0.0153 (14)	0.0032 (11)	−0.0024 (11)	−0.0048 (12)
O7	0.0107 (13)	0.0149 (13)	0.0153 (14)	−0.0019 (11)	−0.0009 (10)	0.0014 (12)
O8	0.0129 (13)	0.0119 (13)	0.0153 (15)	0.0000 (10)	−0.0011 (10)	0.0032 (11)
O9	0.0163 (17)	0.0104 (13)	0.0205 (18)	−0.0026 (11)	−0.0022 (13)	0.0036 (12)
O10	0.0089 (13)	0.0241 (16)	0.0160 (15)	0.0029 (12)	−0.0005 (10)	−0.0028 (12)
O11	0.0167 (14)	0.0088 (13)	0.0104 (14)	−0.0014 (11)	−0.0024 (11)	0.0026 (11)
O12	0.0115 (17)	0.0143 (16)	0.015 (2)	0.0013 (9)	0.0053 (12)	0.0003 (10)
O1W	0.0126 (13)	0.0131 (14)	0.0290 (17)	−0.0034 (11)	0.0055 (12)	−0.0034 (12)

O2W	0.0139 (14)	0.0141 (13)	0.0190 (15)	0.0006 (11)	0.0049 (11)	0.0029 (12)
O3W	0.0349 (17)	0.0137 (14)	0.0172 (15)	0.0030 (12)	0.0059 (13)	0.0009 (12)
O4W	0.0221 (18)	0.0371 (17)	0.0137 (17)	0.0168 (14)	−0.0068 (14)	−0.0093 (14)

Geometric parameters (Å, °)

Ce1—O10	2.449 (2)	S1—O2	1.437 (3)
Ce1—O7	2.465 (3)	S1—O5	1.462 (3)
Ce1—O12^{i}	2.476 (4)	S1—O11	1.498 (3)
Ce1—O11^{ii}	2.517 (3)	S1—O3	1.502 (3)
Ce1—O4W	2.524 (3)	S2—O8	1.460 (3)
Ce1—O3	2.547 (3)	S2—O10	1.463 (3)
Ce1—O3^{i}	2.621 (3)	S2—O6	1.465 (3)
Ce1—O1W	2.647 (3)	S2—O9	1.493 (3)
Ce1—O11	2.710 (3)	S3—O1	1.456 (3)
Ce1—S1	3.2607 (11)	S3—O4	1.463 (3)
Ce2—O1^{iii}	2.354 (3)	S3—O7	1.466 (3)
Ce2—O4^{iv}	2.430 (3)	S3—O12	1.481 (3)
Ce2—O5^{iii}	2.470 (3)	O1—Ce2^{vi}	2.354 (3)
Ce2—O6^{v}	2.489 (3)	O3—Ce1^{i}	2.621 (3)
Ce2—O3W	2.494 (3)	O4—Ce2^{iv}	2.430 (3)
Ce2—O2W	2.497 (3)	O5—Ce2^{vi}	2.470 (3)
Ce2—O9	2.529 (4)	O6—Ce2^{v}	2.489 (3)
Ce2—O8	2.659 (3)	O11—Ce1^{ii}	2.517 (3)
Ce2—S2	3.2143 (9)	O12—Ce1^{i}	2.476 (4)
O10—Ce1—O7	80.99 (9)	O4^{iv}—Ce2—O9	144.23 (11)
O10—Ce1—O12^{i}	135.57 (11)	O5^{iii}—Ce2—O9	78.93 (11)
O7—Ce1—O12^{i}	136.10 (8)	O6^{v}—Ce2—O9	94.03 (10)
O10—Ce1—O11^{ii}	78.49 (9)	O3W—Ce2—O9	80.07 (9)
O7—Ce1—O11^{ii}	143.04 (9)	O2W—Ce2—O9	69.51 (10)
O12^{i}—Ce1—O11^{ii}	77.96 (8)	O1^{iii}—Ce2—O8	75.74 (9)
O10—Ce1—O4W	67.91 (10)	O4^{iv}—Ce2—O8	149.39 (9)
O7—Ce1—O4W	115.31 (11)	O5^{iii}—Ce2—O8	68.43 (9)
O12^{i}—Ce1—O4W	72.81 (13)	O6^{v}—Ce2—O8	76.73 (8)
O11^{ii}—Ce1—O4W	84.61 (10)	O3W—Ce2—O8	123.02 (9)
O10—Ce1—O3	150.11 (9)	O2W—Ce2—O8	110.19 (8)
O7—Ce1—O3	72.45 (8)	O9—Ce2—O8	53.57 (8)
O12^{i}—Ce1—O3	74.32 (10)	O1^{iii}—Ce2—S2	102.43 (7)
O11^{ii}—Ce1—O3	115.47 (8)	O4^{iv}—Ce2—S2	160.40 (8)
O4W—Ce1—O3	136.36 (9)	O5^{iii}—Ce2—S2	70.81 (7)
O10—Ce1—O3^{i}	113.98 (9)	O6^{v}—Ce2—S2	85.72 (6)
O7—Ce1—O3^{i}	69.68 (8)	O3W—Ce2—S2	101.58 (7)
O12^{i}—Ce1—O3^{i}	72.32 (8)	O2W—Ce2—S2	90.50 (6)

O11^{ii}—Ce1—O3^{i}	147.19 (9)	O9—Ce2—S2	26.89 (7)
O4W—Ce1—O3^{i}	73.70 (9)	O8—Ce2—S2	26.70 (6)
O3—Ce1—O3^{i}	69.49 (9)	O2—S1—O5	111.78 (19)
O10—Ce1—O1W	78.08 (9)	O2—S1—O11	112.17 (17)
O7—Ce1—O1W	67.17 (8)	O5—S1—O11	108.23 (17)
O12^{i}—Ce1—O1W	132.17 (10)	O2—S1—O3	110.58 (15)
O11^{ii}—Ce1—O1W	78.67 (9)	O5—S1—O3	109.98 (17)
O4W—Ce1—O1W	144.47 (9)	O11—S1—O3	103.78 (17)
O3—Ce1—O1W	79.12 (8)	O2—S1—Ce1	134.25 (15)
O3^{i}—Ce1—O1W	132.38 (8)	O5—S1—Ce1	113.83 (13)
O10—Ce1—O11	129.81 (9)	O11—S1—Ce1	55.52 (11)
O7—Ce1—O11	111.72 (8)	O3—S1—Ce1	49.18 (10)
O12^{i}—Ce1—O11	67.22 (10)	O8—S2—O10	112.44 (16)
O11^{ii}—Ce1—O11	62.40 (10)	O8—S2—O6	111.47 (16)
O4W—Ce1—O11	132.05 (10)	O10—S2—O6	109.46 (15)
O3—Ce1—O11	53.24 (9)	O8—S2—O9	104.86 (17)
O3^{i}—Ce1—O11	115.95 (7)	O10—S2—O9	109.15 (18)
O1W—Ce1—O11	65.00 (8)	O6—S2—O9	109.32 (19)
O10—Ce1—S1	144.70 (7)	O8—S2—Ce2	54.92 (10)
O7—Ce1—S1	89.84 (6)	O10—S2—Ce2	123.08 (11)
O12^{i}—Ce1—S1	71.67 (9)	O6—S2—Ce2	127.12 (11)
O11^{ii}—Ce1—S1	89.48 (6)	O9—S2—Ce2	50.02 (13)
O4W—Ce1—S1	144.45 (8)	O1—S3—O4	108.98 (17)
O3—Ce1—S1	26.51 (6)	O1—S3—O7	110.62 (16)
O3^{i}—Ce1—S1	94.06 (6)	O4—S3—O7	110.38 (16)
O1W—Ce1—S1	66.99 (6)	O1—S3—O12	108.69 (18)
O11—Ce1—S1	27.09 (6)	O4—S3—O12	108.21 (17)
O1^{iii}—Ce2—O4^{iv}	81.47 (10)	O7—S3—O12	109.91 (19)
O1^{iii}—Ce2—O5^{iii}	82.75 (10)	S3—O1—Ce2^{vi}	159.40 (18)
O4^{iv}—Ce2—O5^{iii}	128.77 (10)	S1—O3—Ce1	104.31 (13)
O1^{iii}—Ce2—O6^{v}	72.44 (10)	S1—O3—Ce1^{i}	138.41 (14)
O4^{iv}—Ce2—O6^{v}	77.08 (10)	Ce1—O3—Ce1^{i}	110.51 (9)
O5^{iii}—Ce2—O6^{v}	141.23 (10)	S3—O4—Ce2^{iv}	148.94 (18)
O1^{iii}—Ce2—O3W	136.83 (10)	S1—O5—Ce2^{vi}	144.59 (18)
O4^{iv}—Ce2—O3W	87.59 (10)	S2—O6—Ce2^{v}	140.98 (15)
O5^{iii}—Ce2—O3W	72.09 (10)	S3—O7—Ce1	138.57 (15)
O6^{v}—Ce2—O3W	144.78 (10)	S2—O8—Ce2	98.38 (13)
O1^{iii}—Ce2—O2W	139.13 (9)	S2—O9—Ce2	103.09 (16)
O4^{iv}—Ce2—O2W	74.93 (9)	S2—O10—Ce1	147.70 (16)
O5^{iii}—Ce2—O2W	137.81 (9)	S1—O11—Ce1^{ii}	144.95 (16)
O6^{v}—Ce2—O2W	70.06 (9)	S1—O11—Ce1	97.39 (12)
O3W—Ce2—O2W	75.42 (9)	Ce1^{ii}—O11—Ce1	117.60 (10)
O1^{iii}—Ce2—O9	129.31 (9)	S3—O12—Ce1^{i}	136.67 (15)

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

Fig. 1

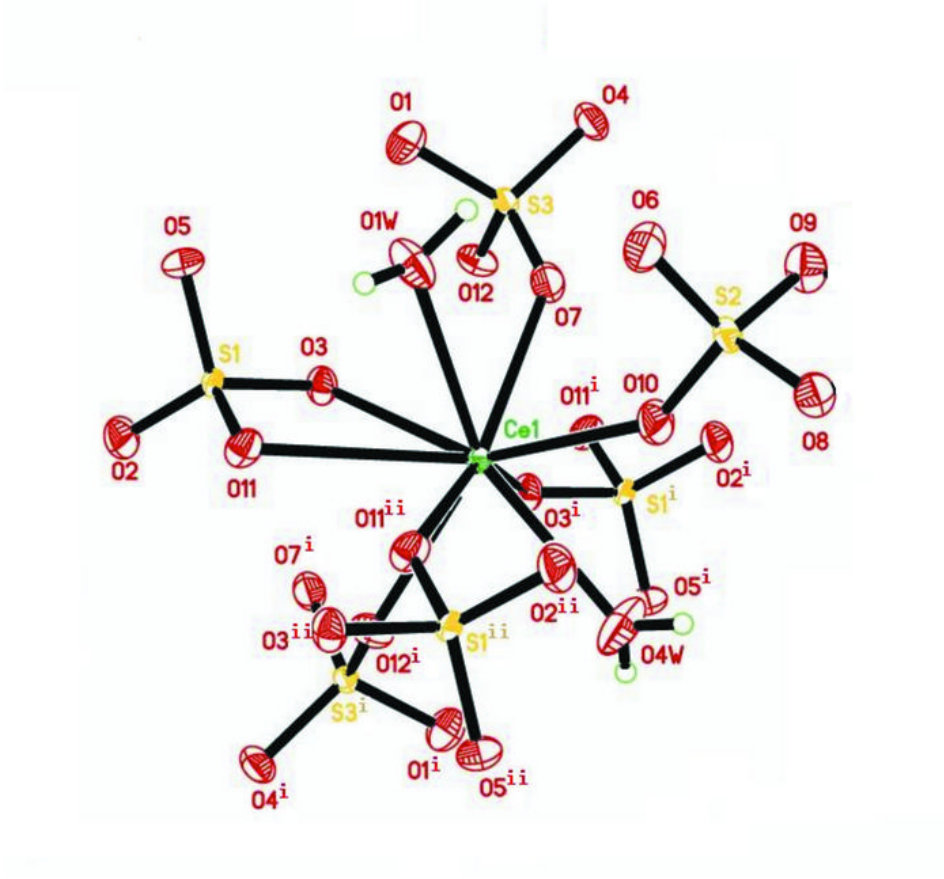

Fig. 2

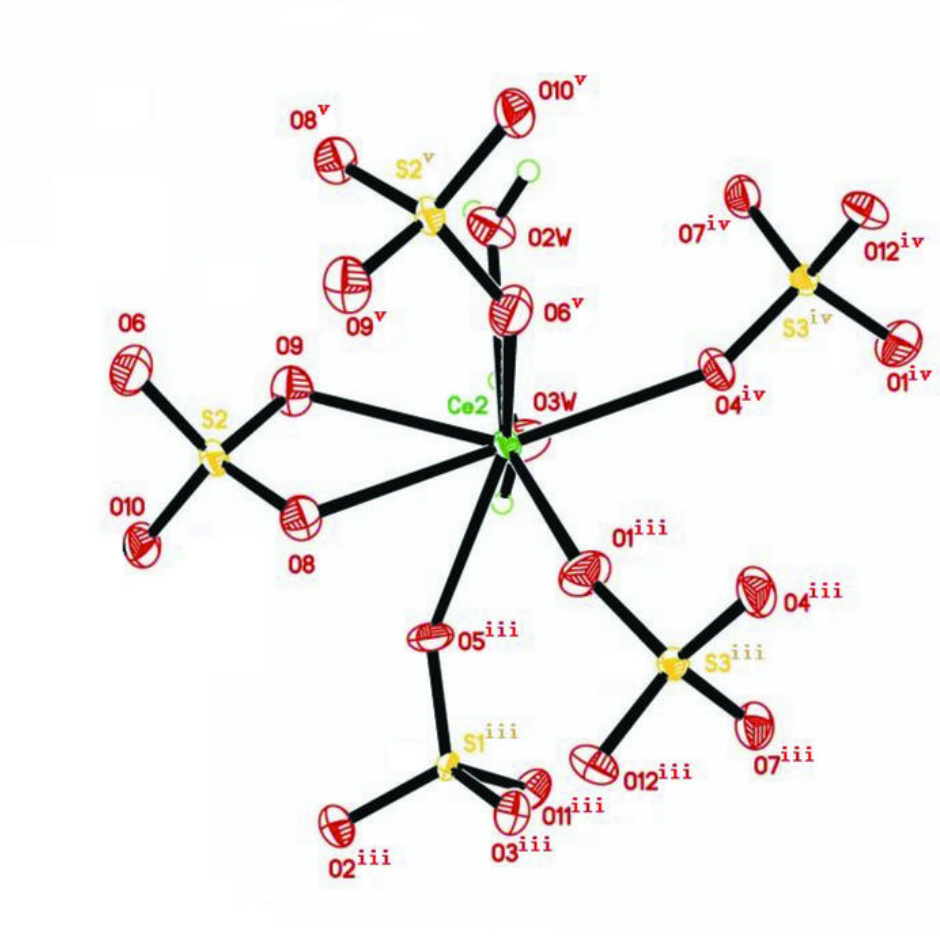
O10v
O8v
S2v
O2W
O7iv
O12iv
O9v
O6v
S3iv
O6
O9
Co2
O3W
O4iv
O1iv
S2
O10
O8
O1iii
O4iii
O5iii
S3iii
S1iii
O12iii
O7iii
O11iii
O3iii
O2iii

Fig. 3