

Scientific paper

A 3D Coordination Polymer of Sm(III) Using Inorganic Sulphate and Organic Succinate Building Blocks

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Abstract

A lanthanide coordination polymeric network, $[\text{Sm}_2(\text{suc})_2(\text{SO}_4)(\text{H}_2\text{O})_2]_n$ (**1**) (suc = succinate dianion), incorporating both organic succinate and inorganic sulphate building blocks, has been synthesized and characterized by single crystal X-ray diffraction analysis. The complex displays a 3D architecture with two crystallographic independent samarium(III) ions having a distorted capped square antiprismatic geometry with O_9 donor set realized by six oxygen atoms from succinate, two from symmetry related sulphate anions and one from an aqua ligand.

Keywords: Coordination polymer, Hydrothermal synthesis, Samarium(III), Succinate, Sulphate

1. Introduction

Lanthanide based coordination polymers are an important class of compounds not only for their potential application as magnetic material,¹ liquid crystals,² luminescent sensors and light converters,^{3,4} but also in biology as agents for molecular-recognition,⁵ or to promote DNA hydrolysis.⁶ In addition lanthanide coordination frameworks present attractive structural topologies^{7–10} and, in continuation of our interest in this field,^{11–13} the combination of organic carboxylate ligands and inorganic species can represent an intriguing subject. In fact tetrahedral XO_4 oxyanions such as silicate,¹⁴ phosphate,¹⁵ arsenate,¹⁶ sulphate,¹⁷ selenate,¹⁸ and borate¹⁹ are well known to act as bridging units not only in inorganic lattices but also in organic-inorganic hybrid compounds. It is evident that these anions do not act simply as a passive constituent but rather contribute to increase the complexity and dimensionality and hence functionality of the network, exerting a synergistic influence at the structure determining organic-inorganic interface. Sulphate is much less reactive compared to phosphate and arsenate but can show versatile coordination modes.¹⁷

Considering the high oxyphilic character of lanthanides, it is expected that the versatile behavior of sulphate ion in conjunction with the flexible coordination of lanthanide ions may lead to a diversity of structural frameworks as exemplified by some amine-templated lanthanum sulphates reported by Louer²⁰ and Rao.²¹ By using succinate dianion we have reported magneto-structural correlation results of a series of isomorphous lanthanide-organic 3D coordination networks, namely $[\text{Ln}^{\text{III}}_2(\text{succinate})_3(\text{H}_2\text{O})_2] \cdot 0.5\text{H}_2\text{O}$ (where Ln = Pr, Nd, Sm, Eu, Gd, and Dy) crystallizing in monoclinic system, space group $I2/a$.¹¹ More recently a Sm succinate compound, of same formulation but containing no lattice water and crystallizing in different lattice system (triclinic, $P\bar{1}$),²² has been described in the literature. Since the potentiality of sulphate in the construction of coordination networks with lanthanide and carboxylate is yet to be explored, we have extended our efforts in the synthesis of lanthanide frameworks that incorporate both organic succinate and inorganic sulphate bridging tectons. Present contribution reports the hydrothermal syntheses and X-ray structural analysis of a three-dimensional Sm(III) coordination polymer of formula $[\text{Sm}_2(\text{suc})_2(\text{SO}_4)(\text{H}_2\text{O})_2]_n$ (**1**) (suc = succinate dianion).

2. Experimental Section

2. 1. Materials and Methods

High purity samarium chloride hexahydrate was purchased from Aldrich Chemical Co. Inc. and used as received. All other chemicals were of AR grade. Elemental analyses (carbon and hydrogen) were performed using a Perkin-Elmer 240C elemental analyzer.

2. 2. Synthesis of $[\text{Sm}_2(\text{suc})_2(\text{SO}_4)(\text{H}_2\text{O})_2] \text{ (1)}$

An aqueous solution (5 mL) of disodium succinate (0.162 g, 1 mmol) was added to an aqueous solution (10 mL) of samarium chloride hexahydrate (0.243 g, 0.66 mmol) under stirring condition. To this mixture solid sodium sulphate decahydrate (0.322 g, 1 mmol) was added and stirred for 30 min. The resultant reaction mixture was transferred to a Teflon-lined steel vessel and heated for 24 h at 175 °C. Light yellow crystals (75% yield) suitable for X-ray analysis were obtained overnight cooling the vessel to room temperature. Found (%): C, 14.44; H, 1.79. Calc for $\text{C}_8\text{H}_{12}\text{Sm}_2\text{SO}_{14}$ (664.94) (%): C, 14.43; H, 1.80.

2. 3. Crystallographic Data Collection, Structure Solution and Refinement

Crystal data and details of data collection and refinement for the structure reported are summarized in

Table 1. Crystallographic data and details of structure refinements for compound **1**

| Compound | 1 |
|--|--|
| Formula | $\text{C}_8\text{H}_{12}\text{Sm}_2\text{SO}_{14}$ |
| Formula weight | 664.94 |
| Crystal system | Monoclinic |
| Space group | $P 2_1/n$ |
| a , Å | 12.846(3) |
| b , Å | 9.632(3) |
| c , Å | 13.027(4) |
| β , ° | 110.24(2) |
| V , Å ³ | 1512.3(7) |
| Z | 4 |
| D_c , g cm ⁻³ | 2.920 |
| μ Mo-K α , mm ⁻¹ | 7.905 |
| $F(000)$ | 1248 |
| θ_{range} (°) | 1.92–31.07 |
| Reflections collected | 22153 |
| Unique reflections | 4821 |
| R_{int} | 0.0268 |
| Observed $I > 2\sigma(I)$ | 4218 |
| Parameters | 238 |
| Goodness of fit (F^2) | 1.051 |
| $R1 / I > 2\sigma(I)$ [a] | 0.0314 |
| $wR2$ [a] | 0.0863 |
| $\Delta\rho / e/\text{Å}^3$ | 0.924, -2.509 [b] |

[a] $R1 = \sum \|F_o\| - \|F_c\| / \sum \|F_o\|$, $wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$

[b] close to Sm1

Table 1. Diffraction data were collected at room temperature on a Nonius DIP-1030H system (Mo-K α radiation, $\gamma = 0.71073$ Å). Cell refinement, indexing and scaling of the data set were carried out using packages Denzo and Scalepack.²³ The structure was solved by direct methods and subsequent Fourier analyses²⁴ and refined by the full-matrix least-squares method based on F^2 with all observed reflections.²⁴ The contribution of H atoms at calculated position (except those of H₂O molecules located on the Δ Fourier map) was introduced in the final cycles of refinement. All the calculations were performed using the WinGX System, Ver 1.80.05.²⁵

3. Results and Discussion

The design of novel coordination networks requires a suitable choice of ligands for their synthesis. The present compound has been synthesized under hydrothermal conditions by using succinate and sulphate anions as ligands since both have versatile coordination modes. The crystalline solid product is stable in air and insoluble in water or common organic solvents such as methanol, acetone and ethanol.

The X-ray diffraction analysis of the compound reveals that the asymmetric unit comprises two Sm(III) ions, two succinate, a sulphate anion and two water molecules. The lanthanide ions present a distorted capped square antiprismatic coordination geometry built by nine oxygen donors, six from succinate, two from symmetry related sulphate anions and an aquo ligand, as shown in Figure 1. Table 2 summarizes the coordination bond lengths, while bond angles are given in Table 1S (supplementary material). The coordination Sm-O distances are close comparable for the two metal ions, varying in the range 2.439(3)–2.677(3) Å and 2.473(3)–2.644(3) Å for Sm(1) and Sm(2), respectively, but no trend has been

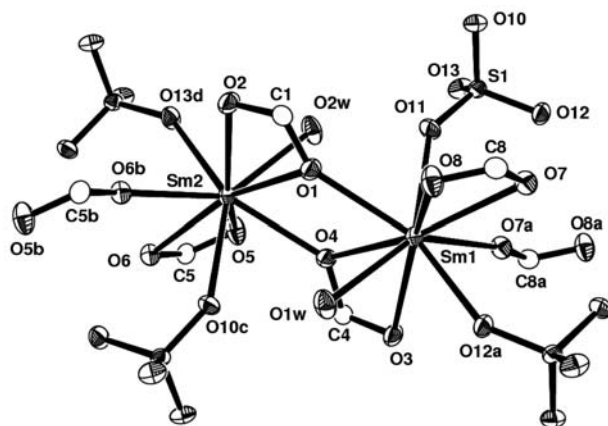


Figure 1. Detail of the 3D structure (ORTEP view) showing the coordination sphere about the two crystallographic independent Sm ions. Symmetry codes: (a) 1-x, 1-y, -z; (b) 1-x, 2-y, 1-z; (c) 1/2+x, 3/2-y, 1/2+z; (d) 1/2-x, 1/2+y, 1/2-z.

Table 2. Selected bond distances (Å) and angles (°) for compound 1.

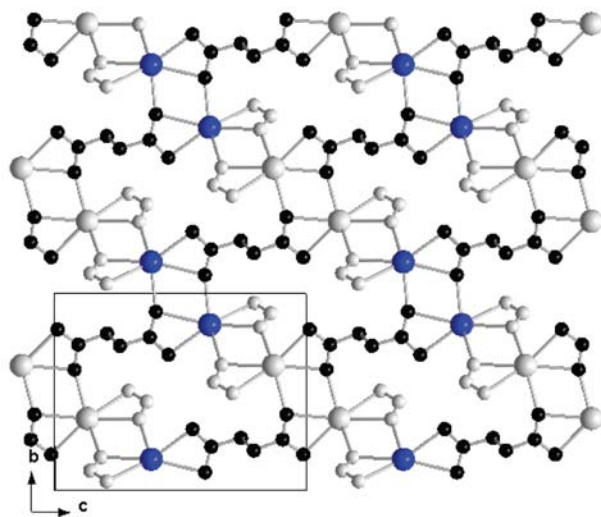
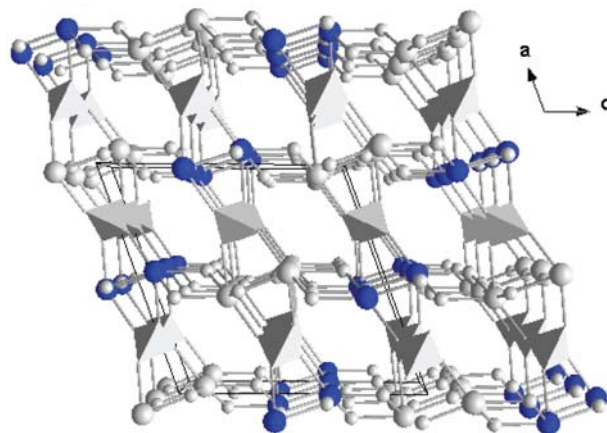
| | | | |
|--------------|----------|--------------|----------|
| Sm(1)–O(1) | 2.547(3) | Sm(2)–O(1) | 2.644(3) |
| Sm(1)–O(3) | 2.609(3) | Sm(2)–O(2) | 2.533(3) |
| Sm(1)–O(4) | 2.586(3) | Sm(2)–O(4) | 2.498(3) |
| Sm(1)–O(7) | 2.677(3) | Sm(2)–O(5) | 2.535(3) |
| Sm(1)–O(7a) | 2.439(3) | Sm(2)–O(6) | 2.579(3) |
| Sm(1)–O(8) | 2.494(3) | Sm(2)–O(6b) | 2.475(3) |
| Sm(1)–O(12a) | 2.472(3) | Sm(2)–O(10c) | 2.588(3) |
| Sm(1)–O(11) | 2.545(3) | Sm(2)–O(13d) | 2.473(3) |
| Sm(1)–O(1w) | 2.518(3) | Sm(2)–O(2w) | 2.498(3) |

Symmetry codes: (a) 1–x, 1–y, –z; (b) 1–x, 2–y, 1–z; (c) 1/2+x, 3/2–y, 1/2+z; (d) 1/2–x, 1/2+y, 1/2–z.

drawn from the oxygen donor type. For comparison the Sm–O coordination distances measured in the two earlier reported $[\text{Sm}_2(\text{suc})_3(\text{H}_2\text{O})_2]_n$ compounds^{11,22} show slightly shorter values varying from 2.346(3) to 2.586(3) Å.

The crystal structure exhibits a 3D polymeric arrangement, which can be described as built up of $[\text{Sm}_2(\text{suc})(\text{H}_2\text{O})_2]_n$ layers, parallel to the *bc* plane, formed by the metals connected *via* bridging succinate ligands C(5)–C(8) (Figure 2). The described layers, separated by half axis *a* (6.423 Å), are further connected by sulphate (having a $\eta^4\mu_4$ coordination mode) and by the other crystallographic independent succinate anion, C(1)–C(4) to give rise to the 3D structure. The connections made by sulphate are depicted in Figure 3, while dicarboxylate anions are intercalated in between the sulphate tetrahedrons (Figure 4).

The two crystallographic independent succinate dianions, involved in the 3D architecture assembly, adopt an *anti* conformation, as indicated by the torsional angles of the carbon skeleton (164.7(3) and 175.3(3)°). However

**Figure 2.** Layer developed in the crystallographic *bc* plane showing the metal arrays (Sm(1) blue, Sm(2) light grey; succinate C(5)–C(8) as black spheres).**Figure 3.** 3D packing viewed down axis *b* (of succinate only bridging oxygen atoms are displayed, tetrahedrons indicate sulphate anions; Sm(1) blue, Sm(2) light grey).

the carboxylate groups are differently oriented with respect to the carbon chains and inside each dianion their mean planes form a dihedral angle of 74.5(1)° in C(1)–C(4), and of 7.6(1)° in the other. This geometrical feature leads to different distances between the chelated lanthanide ions, being 9.394 Å via succinate C(1)–C(4) and 9.587 Å through the C(5)–C(8) spacer. Both the coordinated water molecules (not shown in Figures 2 and 3) are involved in H-bond interactions (Table 3) with a sulphate oxygen and a stronger one with the carboxylate oxygen of the neighbouring layer, thus reinforcing the overall network. The unit cell does not show any residual solvent accessible void.

It is worth noting that the network presents a metal array comparable to those observed in the two Sm succinate derivatives previously reported.^{11,22} In all the structures the samarium ions show a O_9 donor set and a common feature is also represented by arrays of metals where adjacent lanthanide ions are connected by two *syn-anti*

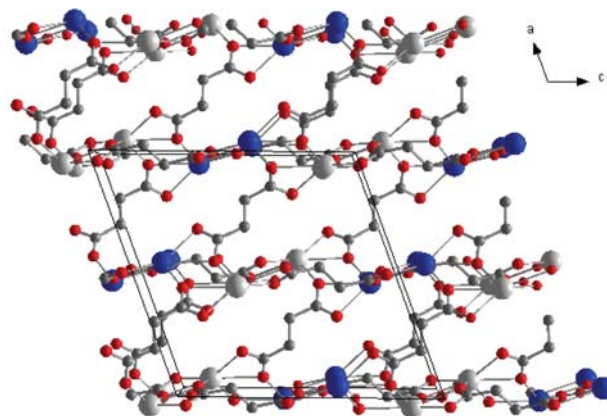
**Figure 4.** 3D packing viewed down axis *b* (sulphate anions not displayed, Sm(1) blue, Sm(2) light grey).

Table 3. Hydrogen bonds involving water molecules in **1**

| D-H | d(D-H) | d(H..A) | <DHA | d(D..A) | A | Symmetry code |
|-------------|--------|---------|--------|---------|-------|----------------------|
| O(1w)-H(11) | 0.869 | 1.854 | 164.71 | 2.702 | O(3) | 3/2-x, 1/2+y, 1/2-z |
| O(1w)-H(10) | 0.893 | 1.964 | 178.60 | 2.857 | O(10) | 1/2+x, 3/2-y, 1/2+z |
| O(2w)-H(21) | 0.907 | 1.774 | 171.69 | 2.674 | O(2) | 1/2-x, -1/2+y, 1/2-z |
| O(2w)-H(20) | 0.888 | 2.028 | 172.25 | 2.911 | O(11) | |

carboxylate groups that are simultaneously chelating and bridging in a $\mu\text{-}\eta^2\text{-}\eta^1$ fashion. Therefore the carboxylate groups chelate one Sm ion and, at the same time, share a chelating oxygen with an adjacent rare earth ion. In addition a bridging carboxylate is operative between the Sm ions in the $[\text{Sm}_2(\text{suc})_3(\text{H}_2\text{O})_2]_n$ compounds while in **1** each pair of Sm(1)₂ and Sm(2)₂ is doubly bridged by two sulphate anions, as depicted in Figure 5 showing a detail of these metal chains. In the present compound the distances between adjacent metal ions are of 4.167(1) Å (Sm(1) ... Sm(1)) and 4.118(1) Å (Sm(2) ... Sm(2)), while slightly longer values are measured in between Sm(1) ... Sm(2), of 4.361(1) Å. In the previously reported structures the lanthanide ions in the line-up were found at slight shorter distance, being equally spaced at 4.085(1) Å¹¹ (one independent metal in this case) or alternated at 4.089 and 4.092 Å.²² Thus the 3D architecture of the present compound is somewhat similar to previously reported structures $[\text{Sm}_2(\text{suc})_3(\text{H}_2\text{O})_2]_n$ formally by replacing a succinate by a sulphate anion, a way that slightly affects the intermetallic distances in the described Sm atom arrays.

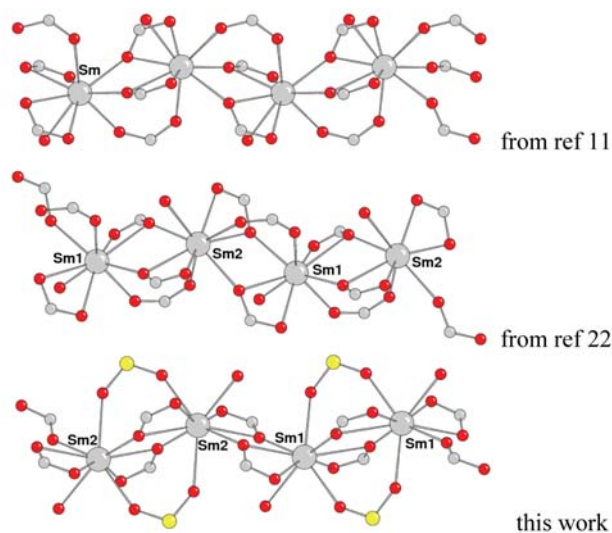


Figure 5. Comparison of metal array in $[\text{Sm}_2(\text{suc})_3(\text{H}_2\text{O})_2]_n$ compounds (see refs 11 and 22) and in the present complex **1**.

4. Conclusions

Hydrothermal reaction of samarium chloride hexahydrate, disodium succinate and sodium sulphate decahydrate resulted a novel 3D organic-inorganic hybrid coordi-

nation polymer, which consists of Sm ions displaying a distorted capped square antiprismatic geometry by nine oxygen atoms. The sulphate anion plays an important role in the formation of the skeleton of the resulting framework, but the metal array present in the structure has comparable features and intermetallic distances to those reported in two previously studied $[\text{Sm}_2(\text{suc})_3(\text{H}_2\text{O})_2]$ derivatives.

5. Acknowledgment

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5. 1. Appendix and Supplementary Material

Crystallographic data reported in this paper has been deposited with the Cambridge Crystallographic Data Center as supplementary publication. CCDC number is 869072. Copy of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: + 44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk). The Table of coordination bond angles of compound **1** has also been deposited as supplementary material.

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Povzetek

Lantanoidna koordinacijska polimerna struktura $[\text{Sm}_2(\text{suc})_2(\text{SO}_4)(\text{H}_2\text{O})_2]_n$ (**1**) (suc = sukcinatni dianion), ki vsebuje tako organske sukcinatne kot anorganske sulfatne enote, je bila sintetizirana in karakterizirana z rentgensko strukturno analizo monokristalov. Kompleks ima tridimenzionalno zgradbo z dvema kristalografsko neodvisnima Sm(III) ionoma, ki sta koordinirana s šestimi kisikovmi atomi iz sukcinatnih, dvema kisikovima atomoma iz sulfatnih anionov in enim, ki pripada akva ligandu.

Supplementary material

Manuscript entitled “A 3D Coordination Polymer of Sm(III) using Inorganic Sulphate and Organic Succinate Building Blocks”

Table 1S. Coordination bond angles (°) of compound 1

| | | | |
|--------------------|------------|---------------------|------------|
| O(1)-Sm(1)-O(3) | 110.57(9) | O(1)-Sm(2)-O(2) | 49.69(9) |
| O(1)-Sm(1)-O(4) | 63.88(9) | O(1)-Sm(2)-O(4) | 63.70(9) |
| O(1)-Sm(1)-O(7) | 115.25(9) | O(1)-Sm(2)-O(5) | 135.55(9) |
| O(1)-Sm(1)-O(7a) | 139.31(10) | O(1)-Sm(2)-O(6) | 160.51(10) |
| O(1)-Sm(1)-O(8) | 77.17(10) | O(1)-Sm(2)-O(6b) | 103.84(9) |
| O(1)-Sm(1)-O(11) | 71.25(10) | O(1)-Sm(2)-O(10c) | 85.90(9) |
| O(1)-Sm(1)-O(12a) | 142.75(10) | O(1)-Sm(2)-O(13d) | 123.43(10) |
| O(1)-Sm(1)-O(1w) | 68.82(11) | O(1)-Sm(2)-O(2w) | 69.48(10) |
| O(3)-Sm(1)-O(4) | 49.82(9) | O(2)-Sm(2)-O(4) | 112.53(9) |
| O(3)-Sm(1)-O(7) | 133.99(9) | O(2)-Sm(2)-O(5) | 147.97(11) |
| O(3)-Sm(1)-O(7a) | 71.96(10) | O(2)-Sm(2)-O(6) | 138.57(9) |
| O(3)-Sm(1)-O(8) | 151.05(11) | O(2)-Sm(2)-O(6b) | 72.27(10) |
| O(3)-Sm(1)-O(1w) | 72.79(11) | O(2)-Sm(2)-O(10c) | 110.56(10) |
| O(3)-Sm(1)-O(11) | 119.29(10) | O(2)-Sm(2)-O(13d) | 78.89(10) |
| O(3)-Sm(1)-O(12a) | 76.23(10) | O(2)-Sm(2)-O(2w) | 76.76(12) |
| O(4)-Sm(1)-O(7) | 160.06(9) | O(4)-Sm(2)-O(5) | 77.57(10) |
| O(4)-Sm(1)-O(7a) | 96.60(9) | O(4)-Sm(2)-O(6) | 107.86(9) |
| O(4)-Sm(1)-O(8) | 139.53(10) | O(4)-Sm(2)-O(6b) | 140.52(10) |
| O(4)-Sm(1)-O(11) | 88.01(10) | O(4)-Sm(2)-O(10c) | 70.33(9) |
| O(4)-Sm(1)-O(12a) | 123.72(10) | O(4)-Sm(2)-O(13d) | 143.18(10) |
| O(4)-Sm(1)-O(1w) | 71.35(10) | O(4)-Sm(2)-O(2w) | 71.27(11) |
| O(7)-Sm(1)-O(7a) | 71.03(11) | O(5)-Sm(2)-O(6) | 50.88(9) |
| O(7)-Sm(1)-O(8) | 50.10(10) | O(5)-Sm(2)-O(6b) | 120.18(10) |
| O(7)-Sm(1)-O(11) | 73.59(9) | O(5)-Sm(2)-O(10c) | 101.47(10) |
| O(7)-Sm(1)-O(12a) | 70.15(10) | O(5)-Sm(2)-O(13d) | 76.52(11) |
| O(7)-Sm(1)-O(1w) | 128.02(10) | O(5)-Sm(2)-O(2w) | 78.37(11) |
| O(7a)-Sm(1)-O(8) | 121.12(10) | O(6)-Sm(2)-O(6b) | 70.90(11) |
| O(7a)-Sm(1)-O(11) | 72.83(10) | O(6)-Sm(2)-O(10c) | 74.62(9) |
| O(7a)-Sm(1)-O(12a) | 77.94(10) | O(6)-Sm(2)-O(13d) | 74.36(10) |
| O(7a)-Sm(1)-O(1w) | 141.59(11) | O(6)-Sm(2)-O(2w) | 126.30(10) |
| O(8)-Sm(1)-O(1w) | 85.21(11) | O(6b)-Sm(2)-O(10c) | 71.54(9) |
| O(8)-Sm(1)-O(11) | 89.66(11) | O(6b)-Sm(2)-O(13d) | 75.88(10) |
| O(8)-Sm(1)-O(12a) | 81.48(11) | O(6b)-Sm(2)-O(2w) | 142.69(11) |
| O(11)-Sm(1)-O(12a) | 139.07(10) | O(10c)-Sm(2)-O(13d) | 140.68(10) |
| O(11)-Sm(1)-O(1w) | 139.89(10) | O(10c)-Sm(2)-O(2w) | 140.62(10) |
| O(12a)-Sm(1)-O(1w) | 79.35(10) | O(13d)-Sm(2)-O(2w) | 78.21(10) |

Symmetry codes: (a) 1-x, 1-y, -z; (b) 1-x, 2-y, 1-z; (c) 1/2+x, 3/2-y, 1/2+z; (d) 1/2-x, 1/2+y, 1/2-z.