

Synthesis and Structures of Nine-Coordinate $\text{K}[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}$ and Ten-Coordinate $\text{K}_2[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2 \cdot 4.5\text{H}_2\text{O}$ Complexes¹

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Abstract—The title complexes, $\text{K}[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}$ (I) (H_4Edta = ethylenediamine- $\text{N},\text{N},\text{N}',\text{N}'$ -tetraacetic acid) and $\text{K}_2[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2 \cdot 4.5\text{H}_2\text{O}$ (II) (H_4Pdta = propylenediamine- $\text{N},\text{N},\text{N}',\text{N}'$ -tetraacetic acid), were prepared and their compositions and structures were determined by elemental analyses and single-crystal X-ray diffraction techniques, respectively. Complex I has a mononuclear structure, and the Sm^{3+} ion is nine-coordinated by an Edta ligand and three water molecules, yielding a pseudo-monocapped square antiprismatic conformation, and the complex crystallizes in the orthorhombic crystal system with space group $Fdd2$. The crystal data are as follows: $a = 19.84(5)$, $b = 35.58(9)$, $c = 12.15(3)$ Å, $V = 8580(38)$ Å³, $Z = 16$, $\rho_c = 1.925$ g/cm³, $\mu = 3.010$ mm⁻¹, $F(000) = 4976$, $R = 0.0252$, and $wR = 0.0560$ for 3510 observed reflections with $I \geq 2\sigma(I)$. Complex II has a binuclear structure and the Sm^{3+} ion is ten-coordinated by a Pdta ligand, two oxygen atoms from a carboxylic group of adjacent Pdta ligand and two water molecules, yielding a distorted bicapped square antiprismatic prism. The complex crystallizes in the triclinic crystal system with space group $P\bar{1}$. The crystal data are as follows: $a = 8.9523(15)$, $b = 10.7106(15)$, $c = 11.6900(19)$ Å, $\alpha = 80.613(5)^\circ$, $\beta = 80.397(5)^\circ$, $\gamma = 76.530(4)^\circ$, $V = 1065.7(3)$ Å³, $Z = 1$, $\rho_c = 1.970$ g/cm³, $\mu = 2.532$ mm⁻¹, $F(000) = 1620$, $R = 0.0332$ and $wR = 0.0924$ for 5390 observed reflections with $I \geq 2\sigma(I)$.

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INTRODUCTION

¹⁵³Sm(III) with an appropriate half-life time and moderate energy, as a radioactive rare-earth metal ion, has attracted much attention of a great number of scientists. The ¹⁵³Sm(III) complexes are widely used for tumor therapy of brain, liver, lung, heart and bone tissues [1–4]. ¹⁵³Sm(III)-ethylenediamine- $\text{N},\text{N},\text{N}',\text{N}'$ -tetramethylenephosphonate (¹⁵³Sm(III)-EDTMP) was first reported as a potential radiopharmaceutical for treatment of bone cancer lesions [5, 6]. This particular radiolabeled chelate emerged as the most promising candidate based on the results of a structure–activity–relationship (SAR) study with a series of multidentate phosphonic acid and multidentate carboxylic acid ligands [7].

Aminopolycarboxylic acids are one kind of multidentate ligands. The ¹⁵³Sm(III) complexes with aminopolycarboxylic acid ligands are used as palliative agents for painful bone metastasis and follow the distribution of radionuclide in vivo [7–9]. These ions should enter

into the body as stable complexes having selectivity and affinity on the focus position and quickly be evacuated from the body after the diagnosis or therapy [4, 9]. Sufficient comprehension of their structures is in favor for researching influence factors of stabilization, thereby for improving. So, it is necessary to study the structure of the Sm(III) complexes with aminopolycarboxylic acid ligands.

In general, the structures or coordination numbers of most metal complexes depend on the ionic radii, electronic configuration, and oxidation state of central metal ions, as well as on the shape of ligands [10–15]. So do rare-earth metal complexes.

Commonly, the rare-earth metal complexes with aminopolycarboxylic acids exist as eight-, nine-, and ten-coordinate forms. For the Sm^{3+} ion with slightly large ionic radius and numbers of f -orbital electrons, as usual, nine-coordinate complexes should be formed. For example, $\text{K}_4[\text{Sm}_2^{\text{III}}(\text{HTtha})_2] \cdot 14\text{H}_2\text{O}$ (H_6Ttha = triethylenetetramine- $\text{N},\text{N},\text{N}',\text{N}',\text{N}'',\text{N}'''$ -hexaacetic acid) is nine-coordinate, adopting a pseudo-monocapped

¹ The article is published in the original.

square antiprism [16], and $\text{Na}_2[\text{Sm}^{\text{III}}(\text{Cydt})][\text{Sm}^{\text{III}}(\text{Cydt})(\text{H}_2\text{O})_3] \cdot 11\text{H}_2\text{O}$ (H_4Cydt = *trans*-1,2-cyclohexanediamine-*N,N,N',N'*-tetraacetic acid) complex has two different parts with the nine-coordinate structure [17]. There are also explanations, however. If the complex could form a binuclear structure with atoms as a bridge, such as an oxygen bridge, the Sm^{3+} ion would have a chance of ten-coordinate structure. Therefore, Edta and Pdta were chosen as ligands to research the structure character of the Sm(III) complexes. They are both six-dentate carboxylic acid ligands. Nevertheless, the Sm(III) complex combining Pdta possesses six-ring rather than five-ring in the Sm(III) complexes combining other aminopolycarboxylic acids such as Edta. This small difference in ligand structure, as we presumed, would induce a distinction of the coordination number and coordination structure. Fortunately, $\text{K}[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}$ (**I**) (H_4Edta is ethylenediamine-*N,N,N',N'*-tetraacetic acid) together with $\text{K}_2[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2 \cdot 4.5\text{H}_2\text{O}$ (**II**) (H_4Pdta is propylenediamine-*N,N,N',N'*-tetraacetic acid) have been synthesized, and their crystal and molecular structures were determined.

EXPERIMENTAL

Synthesis of complexes I. H_4Edta (1.4612 g, 5.0 mmol) was added to 100 ml of warm water, and Sm_2O_3 (0.8718 g, 2.5 mmol) powder was added slowly to the above solution. The solution became transparent after the mixture had been stirred and refluxed for 15.0 h, and then the pH value was adjusted to 6.0 by aqueous KHCO_3 . Finally, the solution was concentrated to 25 ml. A colorless crystal appeared after three weeks at room temperature.

For $\text{C}_{10}\text{H}_{22}\text{N}_2\text{O}_{13}\text{KSm}$

anal. calcd, %: Sm, 26.49; C, 21.15; H, 4.92; N, 4.91; K, 6.90.
Found, %: Sm, 26.48; C, 21.16; H, 3.91; N, 4.93; K, 6.89

This formula is approximately consistent with the result of diffraction analysis.

Synthesis of complexes II. H_4Pdta (1.5313 g, 5.0 mmol) was added to 100 ml of warm water, and Sm_2O_3 (0.8718 g, 2.5 mmol) powder was added to the above solution slowly. The solution became transparent after the mixture had been stirred and refluxed for 15.0 h, and then the pH value was adjusted to 6.0 with aqueous KHCO_3 . Finally, the solution was concentrated to 25 ml. A yellow crystal appeared after three weeks at room temperature.

For $\text{C}_{22}\text{H}_{45}\text{N}_4\text{O}_{24.5}\text{K}_2\text{Sm}_2$

anal. calcd, %: Sm, 26.48; C, 23.23; H, 3.98; N, 4.94; K, 6.90.
Found, %: Sm, 26.46; C, 23.25; H, 3.99; N, 4.93; K, 6.88.

This formula is approximately consistent with the result of diffraction analysis.

The IR spectra of H_4Edta , H_4Pdta , **I** and **II** were determined, respectively, by a Shimadzu-IR 408 spectrophotograph.

X-ray structure determination. X-ray intensity data were collected on a Bruker SMART CCD type X-ray diffractometer system with graphite-monochromatized MoK_α radiation ($\lambda = 0.71073 \text{ \AA}$). The structure was solved by direct methods. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares methods on F^2 . All the calculations were performed by the SHELXTL-97 program on PDP11/44 and Pentium MMX/166 computers. Figures 1 and 2 illustrate the perspective views of complexes **I** and **II**, respectively. Figures 3 and 4 show their coordinating polyhedrons. Figures 5 and 6 show their molecular packings in a unit cell. The crystal data and structure refinement for the two complexes were listed in Table 1. The selected bond distances and bond angles of two complexes are listed in Table 2.

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre (no. 710506 for **I** and 710507 for **II**; deposit@ccdc.cam.ac.uk or <http://www.ccdc.cam.ac.uk>).

RESULTS AND DISCUSSION

A comparison between the infrared spectrum of H_4Edta and that of complex **I** reveals considerable changes due to the coordination. The $\nu(\text{C}-\text{N})$ of **I** is at 1107 cm^{-1} and red-shifts to 27 cm^{-1} comparing with that of H_4Edta (1134 cm^{-1}), which indicates that the nitrogen atoms of H_4Edta coordinated to the Sm(III) atom. The $\nu_{\text{as}}(\text{COOH})$ of H_4Edta at 1689 cm^{-1} disappears, showing that there is no free carboxylic group in complex; the $\nu_{\text{as}}(\text{COO})$ at 1439 cm^{-1} of H_4Edta blue-shifts to 1593 cm^{-1} ; the $\nu_s(\text{COO})$ at 1421 cm^{-1} of H_4Edta red-shifts to 1411 cm^{-1} , which confirms that the oxygen atoms of the carboxyl group coordinate to the Sm(III) atom. There are broad $\nu(\text{OH})$ bands of H_2O near 3388 cm^{-1} revealing the existence of H_2O in the complex.

The $\nu(\text{C}-\text{N})$ of complex **II** is at 1108 cm^{-1} and red-shifts 32 cm^{-1} comparing with that of H_4Pdta (1150 cm^{-1}), which indicates that the nitrogen atoms of H_4Pdta coordinate to Sm(III) atom. The $\nu_{\text{as}}(\text{COOH})$ of H_4Pdta at 1728 cm^{-1} disappears, showing that there is no free carboxylic group in complex, and the $\nu_{\text{as}}(\text{COO})$ at 1660 cm^{-1} of H_4Pdta red-shifts to 1593 cm^{-1} (bridging carboxylic groups) and 1630 cm^{-1} (non-bridging carboxylic groups) [18, 19]. The $\nu_s(\text{COO})$ at 1415 cm^{-1} of H_4Pdta blue-shifts to 1419 cm^{-1} (bridging carboxylic groups) and 1450 cm^{-1} (non-bridging carboxylic groups) in the complex, which confirms that the O atoms of the carboxylic groups coordinate with the Sm^{3+} ions. There are broad $\nu(\text{OH})$ bands of H_2O near

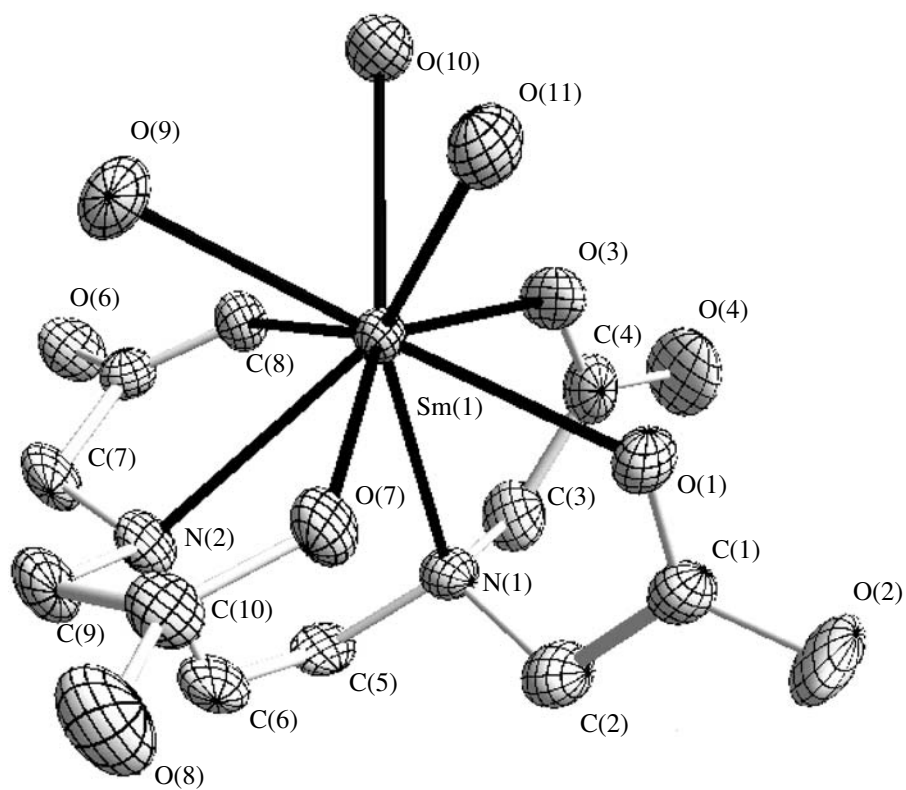


Fig. 1. Molecular structure of complex I.

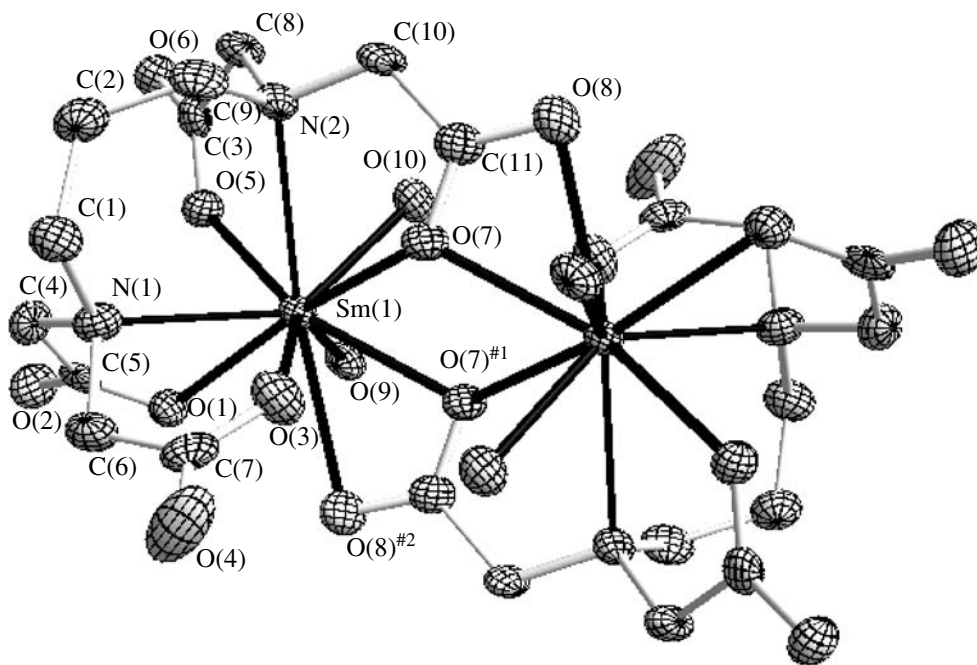


Fig. 2. Molecular structure of complex II.

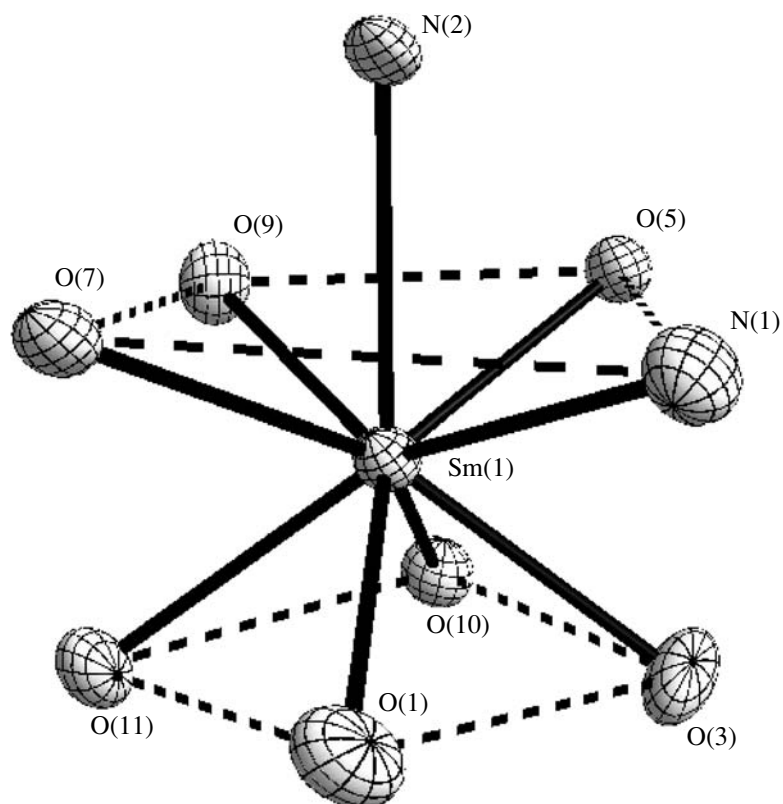


Fig. 3. Coordination polyhedron of complex I.

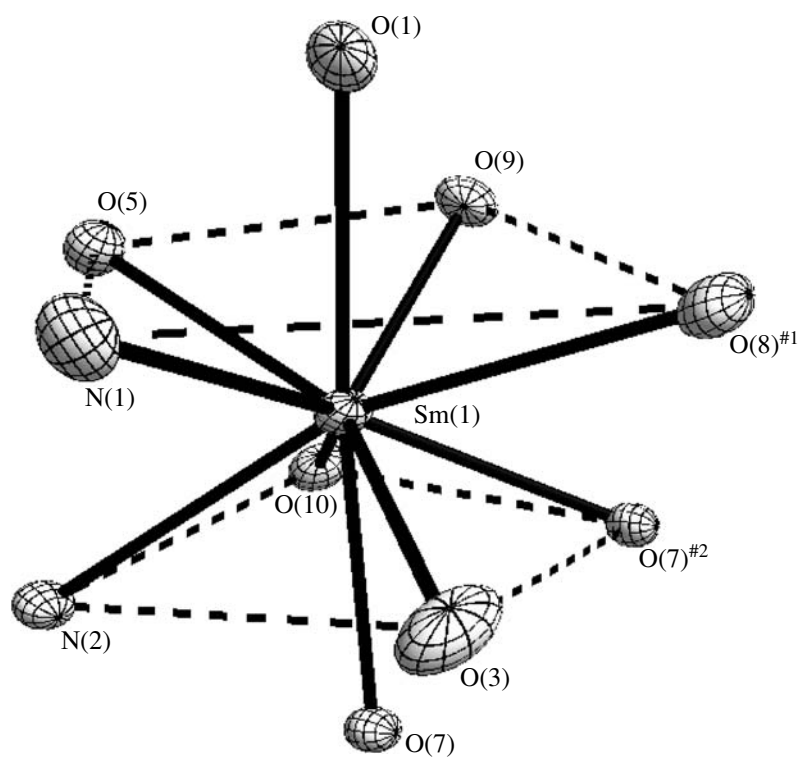


Fig. 4. Coordination polyhedron of complex II.

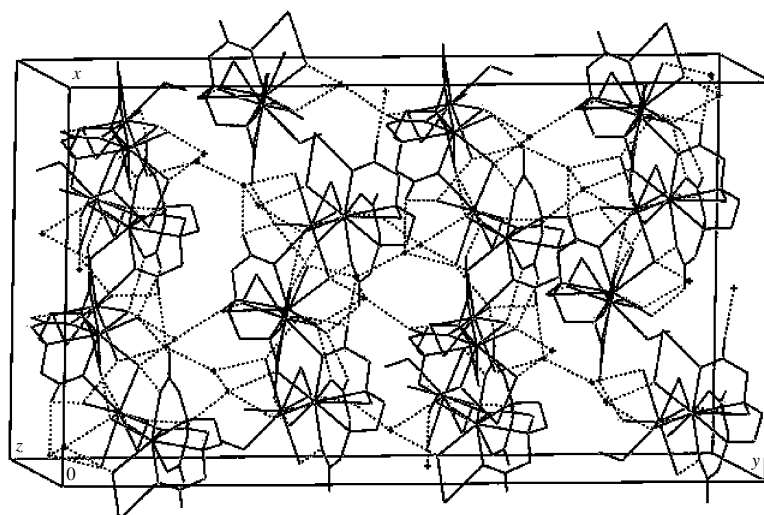


Fig. 5. Arrangement of complex **I** in unit cell (dashed lines represent intermolecular hydrogen bonds).

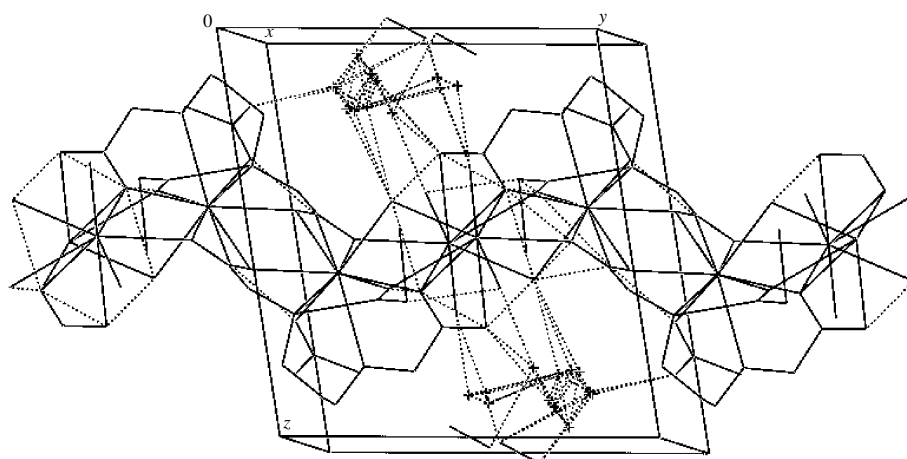


Fig. 6. Arrangement of complex **II** in unit cell (dashed lines represent intermolecular hydrogen bonds).

3435 cm^{-1} revealing the existence of H_2O in the complex.

Figure 1 exhibits the perspective view of the $[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3]^-$ complex anion (in complex **I**). It shows that the Sm^{3+} ion is nine-coordinate by two N and seven O in which three O atoms are from three water molecules and other atoms from one Edta ligand. As shown in Fig. 3, the coordination polyhedron of the $\text{Sm}^{\text{III}}\text{N}_2\text{O}_7$ part adopts the pseudomonocapped square antiprismatic conformation. The set of O(3), O(5), O(9), and O(11) and the set of O(1), O(7), N(1), and N(2) make two approximate parallel square planes. The capped position is occupied by O(10) above the plane of O(3), O(5), O(9), and O(11). The repulsion between the capped atom, O(10), and the top plane formed by O(3), O(5), O(9), and O(11) make the Sm–O(10) bond distance ($2.545(6)\text{ \AA}$) longer than the other Sm–O bond distances, the average distance of which is $2.428(5)\text{ \AA}$. It

also results in the distance between two planes becoming shorter than that of the standard square antiprismatic conformation. Therefore, the conformation of the coordination polyhedron tends to adopt the slightly pseudo one rather than keep standard C_{4v} monocapped square antiprism.

As shown in Fig. 5, in one crystal unit, there are sixteen complex molecules. The $[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3]^-$ complex anions connect with each other by potassium cations and hydrogen bonds, which contribute to stabilizing the crystal structure. Each K^+ cation, as a bridge, links two $[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3]^-$ complex anions. The K^+ cation is coordinated by eight oxygen atoms in which the oxygen atoms from the carboxyl groups of two adjacent Edta ligands and the others from water molecules including three noncoordinated and two coordinated water molecules. Hydrogen bonds in one unit cell link the crystallization water molecules, coordinate

water molecules, and coordinate and noncoordinated O atoms of the Edta ligands. So, a layer structure among the complex molecules in a unit cell is formed through hydrogen bonds and electrostatic actions.

As for complex **II**, its structure is different from that of complex **I**, although there is only one more carbon in the Pdta ligand compared with the Edta ligand. The perspective view of complex **II** shown in Fig. 2, the complex is ten-coordinate with a binuclear molecular structure. Each central Sm^{3+} ion is coordinated by two N and eight O in which six O atoms are from one Pdta ligand, two O from the adjacent Pdta ligand, and the other two O from two water molecules, respectively. The $\text{O}(7)^{\#1}$ and $\text{O}(8)^{\#2}$ atoms are no other than the atoms from the adjacent Pdta ligand, bridging two Sm^{3+} ions and generating a binuclear structure. The $\text{O}(7)^{\#1}$ atom coordinates with two Sm^{III} ions directly, and $\text{O}(8)^{\#2}$, from the same carboxyl group as $\text{O}(7)^{\#1}$, as a big carboxyl group bridge, only coordinates with the adjacent Sm^{3+} ion. The coordination environment around the one Sm^{3+} ion in one molecule is the same as the other one.

As shown in Fig. 4, the coordination polyhedron of $\text{Sm}^{\text{III}}\text{N}_2\text{O}_8$ parts adopts a distorted bicapped square antiprismatic prism. The set of $\text{O}(5)$, $\text{O}(9)$, $\text{O}(8)^{\#2}$, and $\text{N}(1)$, and the set of $\text{O}(3)$, $\text{O}(7)^{\#1}$, $\text{O}(10)$, and $\text{N}(2)$ make two approximate parallel square planes, with torsion angle about 45° . The capping positions are occupied by $\text{O}(1)$ and $\text{O}(7)$ above the plane of $\text{O}(5)$, $\text{O}(9)$, $\text{O}(8)^{\#2}$, and $\text{N}(1)$ and the plane of $\text{O}(3)$, $\text{O}(7)^{\#1}$, $\text{O}(10)$, and $\text{N}(2)$, respectively. It can be found from Table 2 that the bond distances of the Sm^{3+} ion with the capped atoms, $\text{O}(1)$ and $\text{O}(7)$, both are not the longest, being are 2.493(2) and 2.474(2) Å, respectively. As to the top plane, the average bond distance of $\text{Sm}-\text{O}(5)$, $\text{Sm}-\text{O}(9)$, $\text{Sm}-\text{O}(8)^{\#2}$, and $\text{Sm}-\text{N}(1)$ is 2.600(2) Å, with the longest 2.747(3) Å ($\text{Sm}-\text{N}(1)$) and the shortest 2.399(2) Å ($\text{Sm}-\text{O}(5)$). The average bond angle of $\text{O}(1)\text{SmO}(5)$, $\text{O}(1)\text{SmO}(9)$, $\text{O}(1)\text{SmO}(8)^{\#2}$, and $\text{O}(1)\text{SmN}(1)$ is $66.60(7)^\circ$, in which the largest is the $\text{O}(1)\text{SmO}(5)$ bond angle ($69.71(7)^\circ$) and the smallest is the $\text{O}(1)\text{SmN}(1)$ bond angle ($60.77(7)^\circ$). As to the bottom plane, the average bond distance of $\text{Sm}-\text{O}(3)$, $\text{Sm}-\text{O}(7)^{\#1}$, $\text{Sm}-\text{O}(10)$, and $\text{Sm}-\text{N}(2)$ is 2.561(2) Å, with the longest 2.822(2) Å ($\text{Sm}-\text{N}(2)$) and the shortest 2.453(2) Å ($\text{Sm}-\text{O}(3)$). The average bond angle of $\text{O}(7)\text{SmO}(3)$, $\text{O}(7)\text{SmO}(7)^{\#1}$, $\text{O}(7)\text{SmO}(10)$, and $\text{O}(7)\text{SmN}(2)$ is $64.917(8)^\circ$, in which the largest is the $\text{O}(7)\text{SmO}(10)$ bond angle ($70.22(7)^\circ$) and the smallest is the $\text{O}(7)\text{SmN}(2)$ bond angle ($61.31(7)^\circ$). It should be noted that the $\text{O}(1)\text{SmO}(7)$ bond angle is $162.99(7)^\circ$, indicating that the two capped atoms with the metal make not a straight line.

In one unit cell, shown in Fig. 6, there is only one molecule. One $[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2^{2-}$ complex anion contacts with the other $[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2^{2-}$ complex anions by potassium cations and hydrogen bonds, which play an important role in stabilizing the crystal

Table 1. Crystal data and structure refinement for $\text{K}[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}$ (**I**) and $\text{K}_2[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2 \cdot 4.5\text{H}_2\text{O}$ (**II**)

Parameter	Value	
	I	II
Formula weight	621.79	1264.07
Temperature, K	293(2)	293(2)
Crystal system	Orthorhombic	Triclinic
Space group	<i>Fdd2</i>	$P\bar{1}$
Unit cell dimensions:		
<i>a</i> , Å	19.84(5)	8.9523(15)
<i>b</i> , Å	35.58(9)	10.7106(15)
<i>c</i> , Å	12.15(3)	11.6900(19)
β , deg	90	80.397(5)
<i>V</i> , Å ³	8580(38)	1065.7(3)
<i>Z</i>	16	1
ρ_{calc} , mg/cm ³	1.925	1.970
μ , mm ⁻¹	3.010	3.030
<i>F</i> (000)	4976	634
Crystal size, mm	0.25 × 0.20 × 0.20	0.23 × 0.23 × 0.20
θ range for data collection, deg	2.05 to 25.03	3.14 to 27.49
Limiting indices	$-23 \leq h \leq 23$ $-42 \leq k \leq 35$ $-13 \leq l \leq 14$	$-11 \leq h \leq 11$ $-13 \leq k \leq 13$ $-15 \leq l \leq 12$
Reflections collected	8698	8774
Independent reflections	3510 (<i>R</i> _{int} = 0.0295)	4688 (<i>R</i> _{int} = 0.0197)
Completeness to θ_{max} , %	100.0	95.6
Max and min transmission	0.5843 and 0.5199	0.5824 and 0.5386
Goodness-of-fit on <i>F</i> ²	1.052	1.001
Final <i>R</i> indices (<i>I</i> > 2σ(<i>I</i>))	<i>R</i> ₁ = 0.0252, <i>wR</i> ₂ = 0.0560	<i>R</i> ₁ = 0.0243, <i>wR</i> ₂ = 0.0571
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0298, <i>wR</i> ₂ = 0.0571	<i>R</i> ₁ = 0.0260, <i>wR</i> ₂ = 0.0581
Largest difference peak and hole, <i>e</i> Å ⁻³	0.743 and -0.691	1.011 and -0.504
Absorption correction	Semiempirical from equivalents	

Table 2. Selected bond distances and angles of $\text{K}[\text{Sm}^{\text{III}}(\text{Edta})(\text{H}_2\text{O})_3] \cdot 2\text{H}_2\text{O}$ (**I**) and $\text{K}_2[\text{Sm}^{\text{III}}(\text{Pdta})(\text{H}_2\text{O})_2]_2 \cdot 4.5\text{H}_2\text{O}$ (**II**)*

Bond	<i>d</i> , Å	Bond	<i>d</i> , Å	Bond	<i>d</i> , Å
I					
Sm–O(1)	2.400(6)	Sm–O(3)	2.396(6)	Sm–O(5)	2.381(6)
Sm–O(7)	2.437(7)	Sm–O(9)	2.470(6)	Sm–O(10)	2.545(6)
Sm–O(11)	2.483(6)	Sm–N(1)	2.664(7)	Sm–N(2)	2.672(6)
II					
Sm(1)–O(1)	2.493(2)	Sm(1)–O(3)	2.453(2)	Sm(1)–O(5)	2.399(2)
Sm(1)–O(7)	2.474(2)	Sm(1)–O(9)	2.528(2)	Sm(1)–O(10)	2.462(2)
Sm(1)–O(7) ^{#1}	2.507(2)	Sm(1)–O(8) ^{#2}	2.726(2)	Sm(1)–N(1)	2.747(3)
Sm(1)–N(2)	2.822(2)				
Angle	ω, deg	Angle	ω, deg	Angle	ω, deg
I					
O(1)Sm(1)O(3)	70.66(17)	O(1)Sm(1)O(5)	137.69(17)	O(1)Sm(1)O(7)	71.82(13)
O(1)Sm(1)O(9)	142.75(16)	O(1)SmO(10)	118.04(15)	O(1)SmO(11)	74.8(2)
O(3)Sm(1)O(5)	77.0(2)	O(3)Sm(1)O(7)	141.03(18)	O(3)Sm(1)O(9)	139.42(14)
O(3)SmO(10)	70.82(19)	O(3)Sm(1)O(11)	107.83(18)	O(5)Sm(1)O(7)	128.00(14)
O(5)Sm(1)O(9)	79.0(2)	O(5)SmO(10)	73.84(16)	O(5)Sm(1)O(11)	142.69(15)
O(7)Sm(1)O(9)	79.11(17)	O(7)SmO(10)	138.83(14)	O(7)SmO(11)	71.55(15)
O(9)SmO(10)	71.3(2)	O(9)SmO(11)	74.2(2)	O(10)SmO(11)	73.2(2)
O(1)SmN(1)	65.64(17)	O(3)SmN(1)	65.93(14)	O(5)SmN(1)	76.73(16)
O(7)SmN(1)	89.24(15)	O(9)SmN(1)	137.65(17)	O(10)SmN(1)	131.84(18)
O(11)SmN(1)	139.83(17)	O(1)SmN(2)	113.2(2)	O(3)SmN(2)	124.97(17)
O(5)SmN(2)	65.4(2)	O(7)SmN(2)	62.95(16)	O(9)SmN(2)	71.2(2)
O(10)SmN(2)	128.54(17)	O(11)SmN(2)	126.58(19)	N(1)SmN(2)	67.31(18)
II					
O(1)Sm(1)O(3)	97.18(7)	O(1)Sm(1)O(5)	69.71(7)	O(1)Sm(1)O(7)	162.99(7)
O(1)Sm(1)O(9)	67.74(7)	O(1)Sm(1)O(10)	126.53(7)	O(1)Sm(1)O(7) ^{#1}	115.14(7)
O(1)Sm(1)O(8) ^{#2}	68.18(7)	O(3)Sm(1)O(5)	136.28(7)	O(3)Sm(1)O(7)	65.84(7)
O(3)Sm(1)O(9)	137.98(7)	O(3)Sm(1)O(10)	135.66(7)	O(3)Sm(1)O(7) ^{#1}	78.07(7)
O(3)Sm(1)O(8) ^{#2}	69.12(7)	O(5)Sm(1)O(7)	122.77(7)	O(5)Sm(1)O(9)	77.05(7)
O(5)Sm(1)O(10)	74.47(7)	O(5)Sm(1)O(7) ^{#1}	145.59(7)	O(5)Sm(1)O(8) ^{#2}	133.18(7)
O(7)Sm(1)O(9)	123.91(7)	O(7)Sm(1)O(10)	70.22(7)	O(7)Sm(1)O(7) ^{#1}	62.30(8)
O(7)Sm(1)O(8) ^{#2}	102.96(6)	O(9)Sm(1)O(10)	66.48(7)	O(9)Sm(1)O(7) ^{#1}	74.37(7)
O(9)Sm(1)O(8) ^{#2}	68.86(7)	O(10)Sm(1)O(7) ^{#1}	76.81(7)	O(10)Sm(1)O(8) ^{#2}	116.89(7)
O(7) ^{#1} Sm(1)O(8) ^{#2}	49.49(6)	O(1)Sm(1)N(1)	60.77(7)	O(3)Sm(1)N(1)	61.51(7)
O(5)Sm(1)N(1)	76.33(7)	O(7)Sm(1)N(1)	108.59(7)	O(9)Sm(1)N(1)	127.47(7)
O(10)Sm(1)N(1)	142.92(7)	O(7) ^{#1} Sm(1)N(1)	137.17(7)	O(8) ^{#2} Sm(1)N(1)	99.74(7)
O(1)Sm(1)N(2)	124.83(7)	O(3)Sm(1)N(2)	96.45(7)	O(5)Sm(1)N(2)	63.81(7)
O(7)Sm(1)N(2)	61.31(7)	O(9)Sm(1)N(2)	124.73(7)	O(10)Sm(1)N(2)	66.48(7)
O(7) ^{#1} Sm(1)N(2)	119.95(7)	O(8) ^{#2} Sm(1)N(2)	162.77(7)	N(1)Sm(1)N(2)	80.36(7)

* Code symmetry: ^{#1} 1 – *x*, –*y*, 1 – *z*; ^{#2} 1 – *x*, –*y*, 1 – *z*.

structure. Each K^+ cation, as a bridge, connects two $[Sm^{III}(Pdta)(H_2O)_2]_2^{2-}$ complex anions. The K^+ cation is coordinated by eight oxygen atoms in which seven oxygen atoms from the carboxyl groups of two adjacent Pdta ligands including two noncoordinated, five coordinated oxygen atoms, and one from a noncoordinated water molecule. Hydrogen bonds link the crystallization water molecules, coordinate water molecules, and coordinate and noncoordinate O atoms of the Pdta ligands. Therefore, a cage-like structure is formed through hydrogen bonds and electrostatic actions.

Up to now, most complexes of rare-earth metals with Pdta ligand generally form nine-coordinated structures. This complex, however, selects ten-coordinated and binuclear structure, which indicates that it is possible to form the ten-coordinated complex of rare-earth metals with the Pdta ligand, if the central metal ion possesses the slightly big ionic radii and less numbers of f -orbital electrons. The binuclear structure, perhaps, also contributes to a ten-coordinated conformation. Therefore, this work provides the further evidence for our theoretical inferences that the coordination number and coordinated structure of the rare-earth metal complex with aminopolycarboxylic acid ligands depend on the ion radii and electronic configuration of the central metal ion, as well as the shape of the ligand [13, 15, 20, 21].

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