Data Article

Structural data of structure variation and luminescence of 3D, 2D and 1D lanthanide coordination polymers with 1,3-adamantanedicarboxylic acid

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A R T I C L E I N F O

Article history:
Received 20 June 2018
Accepted 24 August 2018
Available online 8 September 2018

A B S T R A C T

In this data article, we report the structure, Fourier transform infrared spectroscopy(FT-IR), powder X-ray diffraction (PARD), luminescence decay, thermogravimetric analysis (TGA) and UV–vis data of three series Ln-MOFs. Detailed structure and luminescence properties were discussed in our previous study (Zhao et al., 2018) [1]. The data includes the structure patterns of ligand H2ADA, FT-IR, PXRD and thermostability of Ln-MOFs in the air, detailed structure information for these structures are listed in Table 1–7.

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Specifications table

| Subject area       | Chemistry |
|--------------------|-----------|
| More specific subject area | Single crystal data of lanthanide complexes |
| Type of data       | Table, figure |

DOI of original article: https://doi.org/10.1016/j.ica.2018.06.027

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How data was acquired
Crystallography open data base and crystallographic tool – Diamond:
Crystallographic Information File Code: 1562086–1562091 1574790.cif
Analyzed

Data format
Single crystal X-ray diffraction data was collected on a Bruker SMART 1000
CCD at 293 K, with Mo-Kα radiation (0.71073 Å). The structure was refined
by full-matrix least-squares methods with SHELXL-97 module. The three
series structures crystalize in orthorhombic space group Pna2₁ (no. 33),
triclinic space group P-1 (no. 2) and monoclinic space group P2(1)/n.

Experimental factors
Single crystal X-ray diffraction data was collected on a Bruker SMART 1000
CCD at 293 K, with Mo-Kα radiation (0.71073 Å). The structure was refined
by full-matrix least-squares methods with SHELXL-97 module. The three
series structures crystalize in orthorhombic space group Pna2₁ (no. 33),
triclinic space group P-1 (no. 2) and monoclinic space group P2(1)/n.

Experimental features
Block colorless single crystals.

Data source location
Jiangxi Normal University, Nanchang, China.

Data accessibility
The data are with this article.

Related research article
Zhi-Peng Zhao, a Kai Zheng, a Hao-Ran Li, a Cheng-Hui Zeng, a,b,d* Shengliang Zhong, a* Seik Weng Ng, d Yanqiong Zheng, d Yun Chen, a Structure Variation and Luminescence of 3D, 2D and 1D Lanthanide
Coordination Polymers with 1,3-Adamantanediacetic Acid, Inorganica
Chimica Acta, revised.

Value of the data
- This data would be valuable for other properties studies of lanthanide complexes that based on
1,3-Adamantanediacetic Acid.
- This data would be valuable for synthesizing lanthanide complexes that coordinated by dmp.
- This data provide a new strategy to control the structure of lanthanide complexes.

1. Data

Three series of lanthanide coordination polymers (Ln-CPs) [1], 3D Ln-CPs [Tb₂(ADA)₃]ₙ (1a, H₂ADA =
1,3-Adamantane-diacetic Acid), 2D Ln-CPs [Ln₂(ADA)₃(dmp)]₂₋ₙ . 2EtOH . H₂O, (Ln³⁺ = Eu³⁺, 2a;
Gd³⁺, 2b; Tb³⁺, 2c; dmp = 4,7-dimethyl-1,10-phenanthroline), and 1D Ln-CPs [Ln(ADA)(HADA)(H₂O)]ₙ
(Ln³⁺ = Eu³⁺, 3a; Gd³⁺, 3b; Tb³⁺, 3c), by using the ligand H₂ADA (Fig. 1). The Ln-CPs are characterized
by single-crystal X-ray diffraction, FT-IR (Figs. 2 and 3), PXRD (Figs. 4 and 5), TGA (Fig. 6) and UV–vis
(Fig. 7). Detailed information about selected bond lengths and angles for 1a, 2a–2c and 3a–3c are listed
in Tables 1–7, they show that the bond lengths and angles are in the normal value as known lanthanide
complexes [2–7].

Fig. 1. Structure of the ligand H₂ADA.
Fig. 2. FT-IR spectra of the ligand and 2a-2c.

Fig. 3. FT-IR spectra of the ligand, 3a and 3c.

Fig. 4. Experimental and calculated PXRD of 2a, 2b and 2c indicate phase purity of the as-synthesized samples.
Fig. 5. PXRD patterns of bulk samples 3a, 3b and 3c compete well with their simulated results of 3a, 3b and 3c, indicating the high phase purity of bulk samples 3a, 3b and 3c.

Fig. 6. a) TGA of 2D Ln-CPs 2a, 2b and 2c in the air atmosphere; b) TGA of 1D Ln-CPs of 3a and 3c in the air atmosphere.

Fig. 7. UV–vis spectrum of solid state sample H₂ADA at room temperature.
Table 1
Selected bond lengths and bond angles of 1a.

| Bond                      | Distance (Å) |
|---------------------------|--------------|
| Tb(1)-O(1)                | 2.248(6)     |
| Tb(1)-O(3)                | 2.263(6)     |
| Tb(1)-O(5)                | 2.267(5)     |
| Tb(1)-O(7)                | 2.325(4)     |
| Tb(1)-O(9)                | 2.331(5)     |
| Tb(1)-O(11)               | 2.562(5)     |
| Tb(1)-O(12)               | 2.389(4)     |
| Tb(1)-Tb(2)               | 3.9029(5)    |
| O(1)-Tb(1)-O(3)           | 173.8(2)     |
| O(1)-Tb(1)-O(5)           | 91.9(2)      |
| O(3)-Tb(1)-O(5)           | 93.2(2)      |
| O(1)-Tb(1)-O(7)           | 86.05(19)    |
| O(3)-Tb(1)-O(7)           | 91.0(2)      |
| O(5)-Tb(1)-O(7)           | 82.02(18)    |
| O(1)-Tb(1)-O(9)           | 91.4(2)      |
| O(3)-Tb(1)-O(9)           | 93.0(2)      |
| O(5)-Tb(1)-O(9)           | 86.05(19)    |
| O(1)-Tb(1)-O(11)          | 90.1(2)      |
| O(3)-Tb(1)-O(11)          | 84.5(2)      |
| O(5)-Tb(1)-O(11)          | 89.3(2)      |
| O(1)-Tb(1)-O(12)          | 90.1(2)      |
| O(3)-Tb(1)-O(12)          | 86.6(2)      |
| O(5)-Tb(1)-O(12)          | 158.2(2)     |
| O(1)-Tb(1)-Tb(2)          | 70.94(16)    |
| O(3)-Tb(1)-Tb(2)          | 103.41(19)   |
| O(5)-Tb(1)-Tb(2)          | 117.52(14)   |
| O(1)-Tb(1)-Tb(2)          | 89.3(2)      |
| O(3)-Tb(1)-Tb(2)          | 88.66(2)     |
| O(5)-Tb(1)-Tb(2)          | 185.2(2)     |
| O(1)-Tb(2)-O(4)           | 102.3(2)     |
| O(3)-Tb(2)-O(4)           | 157.8(2)     |
| O(5)-Tb(2)-O(4)           | 150.87(19)   |
| O(1)-Tb(2)-O(6)           | 83.1(2)      |
| O(3)-Tb(2)-O(6)           | 80.20(11)    |
| O(5)-Tb(2)-O(6)           | 90.55(10)    |
| O(1)-Tb(2)-O(7)           | 124.75(9)    |
| O(3)-Tb(2)-O(7)           | 124.75(9)    |
| O(5)-Tb(2)-O(7)           | 124.75(9)    |

Table 2
Selected bond lengths and bond angles of 2a.

| Bond                      | Distance (Å) |
|---------------------------|--------------|
| Eu(1)-O(8)#1              | 2.358(3)     |
| Eu(1)-O(12)#2             | 2.381(3)     |
| Eu(1)-O(11)#3             | 2.379(3)     |
| Eu(1)-O(10)               | 2.427(3)     |
| Eu(1)-O(7)                | 2.501(3)     |
| Eu(1)-N(4)                | 2.558(4)     |
| Eu(1)-O(8)                | 2.564(3)     |
| Eu(1)-O(9)                | 2.587(3)     |
| Eu(1)-N(3)                | 2.652(4)     |
| O(8)-Eu(1)-O(12)#2        | 77.01(10)    |
| O(8)-Eu(1)-O(11)#3        | 74.13(10)    |
| O(8)-Eu(1)-O(10)          | 88.56(11)    |
| O(8)-Eu(1)-O(7)           | 128.82(10)   |
| O(11)-Eu(1)-O(10)         | 81.14(10)    |
| O(11)-Eu(1)-O(7)          | 124.75(9)    |
| O(11)-Eu(1)-O(4)          | 80.55(10)    |
| O(11)-Eu(1)-O(7)          | 90.85(10)    |
| O(10)-Eu(1)-O(7)          | 142.24(11)   |
| O(8)-Eu(1)-N(4)           | 144.91(11)   |
| O(12)-Eu(1)-N(4)          | 80.23(11)    |
| O(11)-Eu(1)-N(4)          | 138.26(11)   |

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### Table 3
Selected bond lengths and bond angles of 2b.

| Bond Lengths (Å) | Bond Angles (°) |
|------------------|-----------------|
| (1)O(1)-Gd(1)    | 2.341(3)        |
| (1)O(2)-Gd(2)    | 2.367(3)        |
| (1)O(3)-Gd(1)    | 2.372(3)        |
| (1)O(4)-Gd(1)    | 2.418(3)        |
| (1)O(5)-Gd(2)    | 2.494(3)        |
| (1)N(1)-Gd(1)    | 2.546(3)        |
| (1)O(6)-Gd(1)    | 2.560(2)        |
| (1)O(7)-Gd(1)    | 2.584(3)        |
| (1)N(2)-Gd(1)    | 2.641(4)        |
| (1)O(8)-Gd(2)    | 74.36(9)        |
| (1)Gd(1)-O(12)   | 77.01(9)        |
| (1)Gd(1)-O(11)   | 137.46(8)       |
| (1)Gd(1)-O(10)   | 88.69(10)       |
| (1)Gd(2)-Gd(1)   | 129.04(10)      |
| (1)Gd(1)-O(7)    | 124.92(8)       |
| (1)Gd(1)-O(6)    | 90.75(9)        |
| (1)Gd(1)-O(5)    | 80.56(10)       |
| (1)Gd(1)-O(4)    | 141.94(10)      |
| (1)Gd(1)-Gd(2)   | 144.54(11)      |
| (1)Gd(2)-O(1)    | 138.45(11)      |
| (1)Gd(2)-O(4)    | 79.90(10)       |
| (1)Gd(1)-N(1)    | 85.31(10)       |
| (1)Gd(1)-N(1)    | 76.44(10)       |
| (1)Gd(2)-O(8)    | 73.91(10)       |
| (1)Gd(1)-O(12)   | 71.58(8)        |
| (1)Gd(1)-O(10)   | 70.66(6)        |
| (1)Gd(1)-O(8)    | 150.61(9)       |
| (1)Gd(1)-O(9)    | 51.21(8)        |
| (1)Gd(1)-N(1)    | 122.49(9)       |
| (1)Gd(1)-N(1)    | 80.14(9)        |
| (1)Gd(1)-O(6)    | 126.29(9)       |
| (1)Gd(1)-O(5)    | 77.71(9)        |
| (1)Gd(1)-N(1)    | 51.55(9)        |
| (1)Gd(1)-N(1)    | 141.57(9)       |
| (1)Gd(1)-N(1)    | 68.83(10)       |
| (1)Gd(1)-N(1)    | 142.65(9)       |
| (1)Gd(1)-N(1)    | 146.01(10)      |
| (1)Gd(1)-N(1)    | 75.87(10)       |
| (1)Gd(1)-N(1)    | 136.95(10)      |

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y, z; #2 x+1, y, z; #3 -x+1, -y, -z+1; #4 x+2, -y+1, -z; #5 -x+3, -y+1, -z; #6 x+1, y, z.
2. Experimental design, materials, and methods

Synthesis of 1a: In a 250 mL Teflon-lined stainless-steel autoclave, 0.396 mmol H₂ADA, 0.594 mmol Tb(NO₃)₃·6H₂O and 0.396 mmol 1,10-phenanthroline (phen) were mixed, then 100 mL H₂O added, and mixed by a magnetic stirrer. The reactants were sealed in the Teflon-lined stainless-steel autoclave and heated at 418 K for 6 days.

Synthesis of 2a–2c: In a 50 mL beaker, 0.396 mmol H₂ADA and 20 mL H₂O were mixed, and the pH adjusted to 6 with 0.1 M NaOH solution. Then the solution was mixed with 20 mL MeOH solution containing 0.27 mmol Ln(NO₃)₃·6H₂O. After that, 0.269 mmol dmp dissolved in 20 mL EtOH solution was added to the mixture. Then it was transferred to a bottle and sealed, allowing the reaction to proceed at 333 K for 72 h.

Synthesis of 3a–3c: In a 100 mL bottle, 0.396 mmol H₂ADA was mixed with 0.13 mmol Ln(NO₃)₃·6H₂O. 10 mL DMF and 50 mL H₂O was added and stirred for 10 min. Then the bottle was sealed and reacted at 333 K for 72 h.

Table 4
Selected bond lengths and bond angles of 2c.

| Bond | Length/Å | Angle/° |
|------|----------|---------|
| Tb(1)-O(2)#1 | 2.335(2) | O(3)-Tb(2)-O(10) |
| Tb(1)-O(6)#1 | 2.352(2) | O(1)-Tb(2)-O(10) |
| Tb(1)-O(5) | 2.352(2) | O(1)-Tb(2)-O(10) |
| Tb(1)-O(7)#2 | 2.400(3) | Tb(2)-O(9)#3 |
| Tb(1)-O(1) | 2.484(3) | Tb(2)-O(4)#3 |
| Tb(1)-N(1) | 2.525(3) | Tb(2)-O(11)#4 |
| Tb(1)-O(2) | 2.550(2) | Tb(2)-O(12)#4 |
| Tb(1)-N(2) | 2.624(3) | Tb(2)-N(3) |
| O(2)#1-Tb(1)-O(6)#1 | 74.52(9) | O(3)-Tb(2)-O(10) |
| O(2)#1-Tb(1)-O(5) | 77.01(9) | O(3)-Tb(2)-O(10) |
| O(2)#1-Tb(1)-O(7)#2 | 88.32(10) | O(3)-Tb(2)-O(4)#3 |
| O(2)#1-Tb(1)-O(1) | 125.17(8) | O(3)-Tb(2)-O(4)#3 |
| O(2)#1-Tb(1)-N(1) | 144.25(10) | O(3)-Tb(2)-O(4)#3 |
| O(2)#1-Tb(1)-O(2) | 74.05(9) | O(3)-Tb(2)-O(4)#3 |

Symmetry transformations used to generate equivalent atoms: #1 x+1, y+2, z; #2 x+1, y, z; #3 x+1, y+3, z+1; #4 -x+2, -y+3, -z+1; #5 x-1, y, z.

2. Experimental design, materials, and methods

Synthesis of 1a: In a 250 mL Teflon-lined stainless-steel autoclave, 0.396 mmol H₂ADA, 0.594 mmol Tb(NO₃)₃·6H₂O and 0.396 mmol 1,10-phenanthroline (phen) were mixed, then 100 mL H₂O added, and mixed by a magnetic stirrer. The reactants were sealed in the Teflon-lined stainless-steel autoclave and heated at 418 K for 6 days.

Synthesis of 2a–2c: In a 50 mL beaker, 0.396 mmol H₂ADA and 20 mL H₂O were mixed, and the pH adjusted to 6 with 0.1 M NaOH solution. Then the solution was mixed with 20 mL MeOH solution containing 0.27 mmol Ln(NO₃)₃·6H₂O. After that, 0.269 mmol dmp dissolved in 20 mL EtOH solution was added to the mixture. Then it was transferred to a bottle and sealed, allowing the reaction to proceed at 333 K for 72 h.

Synthesis of 3a–3c: In a 100 mL bottle, 0.396 mmol H₂ADA was mixed with 0.13 mmol Ln(NO₃)₃·6H₂O. 10 mL DMF and 50 mL H₂O was added and stirred for 10 min. Then the bottle was sealed and reacted at 333 K for 72 h.
The lanthanide salts were obtained by the procedures as our previous work [8–13]. H$_2$ADA (97.0%) was purchased from Innochem (Beijing, China) and used without any purification. Other chemicals (A.R.) are commercially available and were used as received.

Single crystal X-ray diffraction data was collected on a Bruker SMART 1000 CCD, with Mo-Ka radiation (Wavelength = 0.71073 Å) at room temperature. The structure was refined by full-matrix least-squares methods with SHELXL-97 module. FT-IR was obtained in KBr pellets and recorded on a Nicolet 330 FT-IR spectrometer. TGA was recorded on a Netzsch-Bruker TG-209 unit in the air atmosphere. Luminescence spectra and lifetimes were recorded on an Edinburgh FLS980 at room temperature. Phase purity of bulk sample was determined on a DMAX2200VPC diffractometer, at 30 kV and 30 mA.

Table 5
Selected bond lengths and bond angles of 3a.

|                  | Eu(1)-O(6)#1 | Eu(1)-O(2) | Eu(1)-O(3)#1 |
|------------------|--------------|------------|--------------|
| Eu(1)-O(5)       | 2.296(3)     | Eu(1)-O(1) | 2.610(2)     |
| Eu(1)-O(2)#2     | 2.377(2)     | Eu(1)-Eu(1)#2 | 4.1260(3) |
| Eu(1)-O(9)       | 2.377(2)     | Eu(1)-O(4)#1 | 2.488(2)    |
| Eu(1)-O(3)#1     | 2.415(2)     | Eu(1-O(1)  | 2.421(2)     |
| O(6)#1-Eu(1)-O(5)| 98.94(9)     | O(3)#1-Eu(1)-O(1)| 155.20(8) |
| O(6)#1-Eu(1)-O(2)#2 | 165.00(9) | O(6)#1-Eu(1)-O(4)#1 | 78.02(9) |
| O(5)-Eu(1)-O(9)  | 108.01(9)    | O(2)#2-Eu(1)-O(4)#1 | 91.69(8)   |
| O(5)-Eu(1)-O(9)  | 145.34(8)    | O(9)-Eu(1)-O(4)#1 | 73.82(7)    |
| O(2)#2-Eu(1)-O(9)| 78.98(8)     | O(3)#1-Eu(1)-O(4)#1 | 53.17(8)   |
| O(6)#1-Eu(1)-O(3)#1 | 84.76(9) | O(1)-Eu(1)-O(4)#1 | 133.18(8)  |
| O(5)-Eu(1)-O(3)#1 | 81.27(8)     | O(6)#1-Eu(1)-O(2) | 125.99(8)  |
| O(2)#2-Eu(1)-O(3)#1 | 80.32(8) | O(5)-Eu(1)-O(2) | 73.93(7)    |
| O(9)-Eu(1)-O(3)#1 | 121.82(8)    | O(2)#2-Eu(1)-O(2) | 68.44(8)    |
| O(6)#1-Eu(1)-O(1) | 75.15(9)     | O(9)-Eu(1)-O(2) | 72.67(9)    |
| O(5)-Eu(1)-O(1)  | 87.55(8)     | O(6)#1-Eu(1)-O(2) | 142.62(8)  |
| O(2)#2-Eu(1)-O(1) | 119.66(8)   | O(1)-Eu(1)-O(2) | 51.47(7)    |
| O(9)-Eu(1)-O(1)  | 78.96(8)     | O(4)#1-Eu(1)-O(2) | 143.66(7)  |

Symmetry transformations used to generate equivalent atoms: #1 $-x+2$, $-y+1$, $-z$; #2 $-x+1$, $-y+1$, $-z$.

Table 6
Selected bond lengths and bond angles of 3b.

|                  | Gd(1)-O(6)#1 | Gd(1)-O(3)#1 | Gd(1)-O(2) |
|------------------|--------------|--------------|------------|
| Gd(1)-O(5)       | 2.2839(19)   | Gd(1)-O(1)  | 2.409(2)   |
| Gd(1)-O(4)#2     | 2.3658(17)   | Gd(1)-O(4)#1 | 2.599(18)  |
| Gd(1)-O(1#1)     | 2.3641(18)   | Gd(1)-O(1)  | 2.4069(19)|
| O(6)#1-Gd(1)-O(5)| 98.54(7)     | O(1)-Gd(1)-O(3)#1 | 154.83(7) |
| O(6)#1-Gd(1)-O(4)#2 | 164.99(7) | O(6)#1-Gd(1)-O(2) | 77.98(7)   |
| O(5)-Gd(1)-O(4)#2 | 80.77(6)     | O(5)-Gd(1)-O(2) | 134.30(6)  |
| O(6)#1-Gd(1)-O(1#1) | 108.48(7) | O(4)#2-Gd(1)-O(2) | 91.70(7)   |
| O(5)-Gd(1)-O(1#1) | 145.49(6)    | O(1#1)-Gd(1)-O(2) | 73.75(6)   |
| O(4)#2-Gd(1)-O(1#1) | 78.44(7) | O(1)-Gd(1)-O(2) | 53.36(6)   |
| O(6)#1-Gd(1)-O(1#1) | 84.59(7) | O(3)#1-Gd(1)-O(2) | 133.25(7)  |
| O(5)-Gd(1)-O(1#1) | 80.96(7)     | O(6)#1-Gd(1)-O(4)#1 | 126.04(6) |
| O(4)#2-Gd(1)-O(1#1) | 80.48(6) | O(5)-Gd(1)-O(4)#1 | 74.01(6)   |
| O(1#1)-Gd(1)-O(4)#1 | 121.79(7) | O(4)#2-Gd(1)-O(4)#1 | 68.38(7)   |
| O(6)#1-Gd(1)-O(3)#1 | 75.13(7) | O(1#1)-Gd(1)-O(4)#1 | 72.83(6)   |
| O(5)-Gd(1)-O(3)#1 | 119.66(8)    | O(1#1)-Gd(1)-O(4)#1 | 51.55(6)   |
| O(4)#2-Gd(1)-O(3)#1 | 79.49(7) | O(4)#1-Gd(1)-O(4)#1 | 143.82(6)  |

Symmetry transformations used to generate equivalent atoms: #1 $-x+1$, $-y+1$, $-z$; #2 $-x+1$, $y$, $z$; #3 $x+1$, $y$, $z$. 

The lanthanide salts were obtained by the procedures as our previous work [8–13]. H$_2$ADA (97.0%) was purchased from Innochem (Beijing, China) and used without any purification. Other chemicals (A.R.) are commercially available and were used as received.
Acknowledgments

This study was funded by the National Natural Science Foundation of China (Nos. 21641008 and 91622105), Jiangxi Provincial Department of Science and Technology (Nos. 20151BDH80049 and 20161BAB203083), Jiangxi Provincial Education Department (No. GJJ14259), National Undergraduate Innovation and Entrepreneurship Training Program of China (201710414001), Graduate Innovation Fund of Jiangxi Province (YC2017-S130).

Transparency document. Supplementary material

Transparency document associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2018.08.148.

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Table 7
Selected bond lengths and bond angles of 3c.

| Bond Lengths and Angles | Symmetry Transformations |
|------------------------|--------------------------|
| Tb(1)-O(2)#1           | Tb(1)-O(2)#1             |
| Tb(1)-O(0AA)           | Tb(1)-O(0AA)             |
| Tb(1)-O(5)             | Tb(1)-O(5)               |
| Tb(1)-O(1W)            | Tb(1)-O(1W)              |
| O(2)#1-Tb(1)-O(0AA)    | O(2)#1-Tb(1)-O(0AA)      |
| O(2)#2-Tb(1)-O(5)      | O(2)#2-Tb(1)-O(5)        |
| O(2)#3-Tb(1)-O(1W)     | O(2)#3-Tb(1)-O(1W)       |
| O(5)-Tb(1)-O(1W)       | O(5)-Tb(1)-O(1W)         |
| O(5)#1-Tb(1)-O(0AA)    | O(5)#1-Tb(1)-O(0AA)      |
| O(5)#2-Tb(1)-O(5)      | O(5)#2-Tb(1)-O(5)        |
| O(5)#3-Tb(1)-O(1W)     | O(5)#3-Tb(1)-O(1W)       |
| O(5)#4-Tb(1)-O(0AA)    | O(5)#4-Tb(1)-O(0AA)      |
| O(5)#5-Tb(1)-O(5)      | O(5)#5-Tb(1)-O(5)        |
| O(5)#6-Tb(1)-O(1W)     | O(5)#6-Tb(1)-O(1W)       |
| O(5)#7-Tb(1)-O(0AA)    | O(5)#7-Tb(1)-O(0AA)      |
| O(5)#8-Tb(1)-O(5)      | O(5)#8-Tb(1)-O(5)        |
| O(5)#9-Tb(1)-O(1W)     | O(5)#9-Tb(1)-O(1W)       |

Symmetry transformations used to generate equivalent atoms: #1 –x+1, –y+1, –z; #2 x+1, y, z; #3 –x, –y+1, –z; #4 x–1, y, z.