

**Keywords:** alkaline earth complexes; tetrazol-carboxylate coordination compounds; *in situ* synthesis; photoluminescence; TGA; FT-IR; topology; crystal structure.

**CCDC references:** 2003538; 2003537

**Supporting information:** this article has supporting information at journals.iucr.org/e

# *In situ* synthesis, crystal structures, topology and photoluminescent properties of poly[di- $\mu$ -aqua-diaqua[ $\mu_3$ -4-(1*H*-tetrazol-1-ido-5-yl)benzoato- $\kappa^4$ O:O,O':O'']barium(II)] and poly[ $\mu$ -aqua-diaqua[ $\mu_3$ -4-(1*H*-tetrazol-1-ido-5-yl)benzoato- $\kappa^4$ O:O,O':O'']strontium(II)]

Mohamed Abdellatif Bensegueni,\* Aouatef Cherouana and Hocine Merazig

Environmental, Molecular and Structural Chemistry Research Unit, University of Constantine-1, 25000, Constantine, Algeria. \*Correspondence e-mail: bensegueni.abdellatif@gmail.com

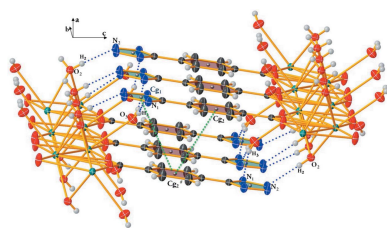
Two alkaline-earth coordination compounds, [Ba(C<sub>8</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>)(H<sub>2</sub>O)<sub>4</sub>]<sub>n</sub>, (I), and [Sr(C<sub>8</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>)(H<sub>2</sub>O)<sub>3</sub>]<sub>n</sub>, (II), from the one-pot hydrolysis transformation of benzoyl chloride and the *in situ* self-assembled [2 + 3] cycloaddition of nitrile are presented. These coordination compounds are prepared by reacting 4-cyanobenzoyl chloride with divalent alkaline-earth salts (BaCl<sub>2</sub> and SrCl<sub>2</sub>) in aqueous solution under hydrothermal conditions. The mononuclear coordination compounds (I) and (II) show the same mode of coordination of the organic ligands. The cohesion of the crystalline structures is provided by hydrogen bonds and  $\pi$ -stacking interactions, thus forming three-dimensional supramolecular networks. The two compounds have a three-dimensional (3,6)-connected topology, and the structural differences between them is in the number of water molecules around the alkaline earth metals. Having the same emission frequencies, the compounds exhibit photoluminescence properties with a downward absorption value from (I) to (II).

## 1. Chemical context

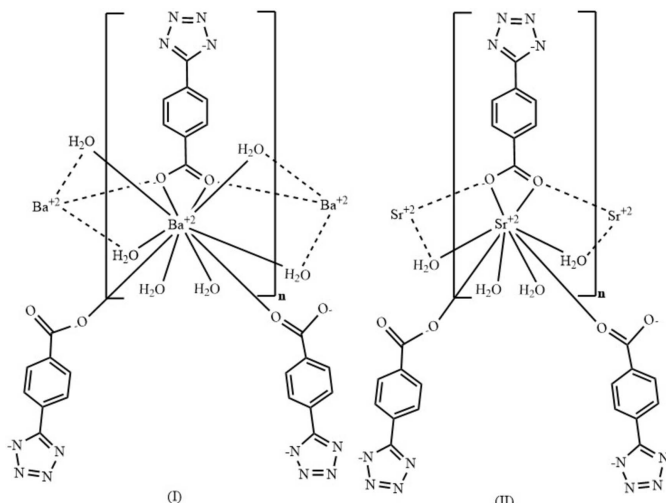
In recent years, studies on a wide variety of tetrazolyl-5-substituted coordination compounds have proliferated (Klapötke & Stierstorfer, 2009; Fischer *et al.*, 2011). The extension from the synthetic approach developed by Demko and Sharpless (2001) to that of Zhao and colleagues (Zhao *et al.*, 2008) is the main reason for this new interest. Chemists have focused on transition-metal compounds, while studies with alkaline-earth metal-tetrazol coordination compounds remain scarce. This led us to further explore this type of compound, and to study their topological and physical properties.

The choice of ligand is essential in the design of new coordination compounds. In our study we selected a (tetrazol-carboxylate) bifunctional ligand, which is able to adopt several coordination modes, resulting in a variety of crystal structures (Ouellette *et al.*, 2012; Sun *et al.*, 2013; Wei *et al.*, 2012).

The complexation and formation of both the tetrazole and carboxylate groups occurred *in situ* under hydrothermal conditions from a 4-cyano-benzoyl chloride and the alkaline earth salts BaCl<sub>2</sub>·2H<sub>2</sub>O and SrCl<sub>2</sub>·6H<sub>2</sub>O, giving the title compounds poly[di- $\mu$ -aqua-diaqua[ $\mu_3$ -5-(4-carboxylatophenyl)-1*H*-1,2,3,4-tetrazol-1-ido- $\kappa^4$ O:O,O':O'']barium(II)] (I)

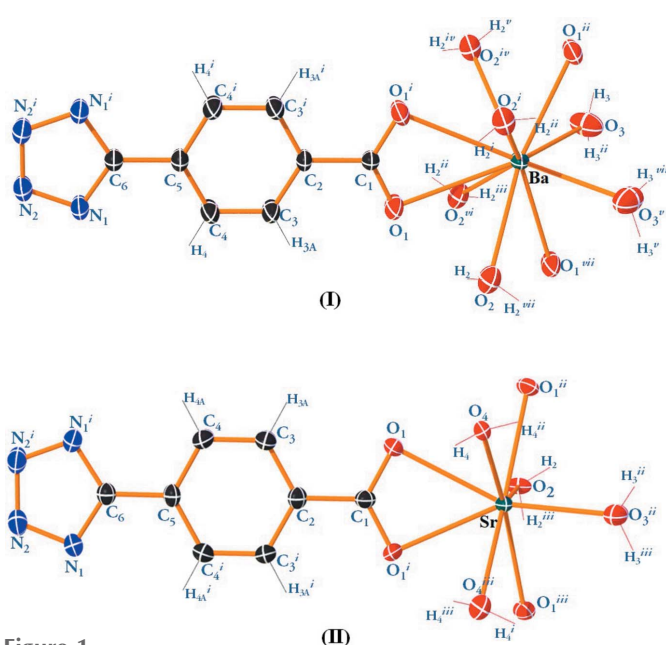


and poly[ $\mu$ -aqua-diaqua[ $\mu_3$ -4-(1*H*-tetrazol-1-yl-5-yl)benzoato- $\kappa^4$ O:O,O':O']strontium(II)] (II). The two compounds form one-dimensional crystalline chains, in which the coordination is ensured by chelating carboxylate groups. The two compounds were characterized by FT-IR, TGA and single-crystal X-ray diffraction analysis. A topological study was performed and the photoluminescent properties were also studied.



## 2. Structural commentary

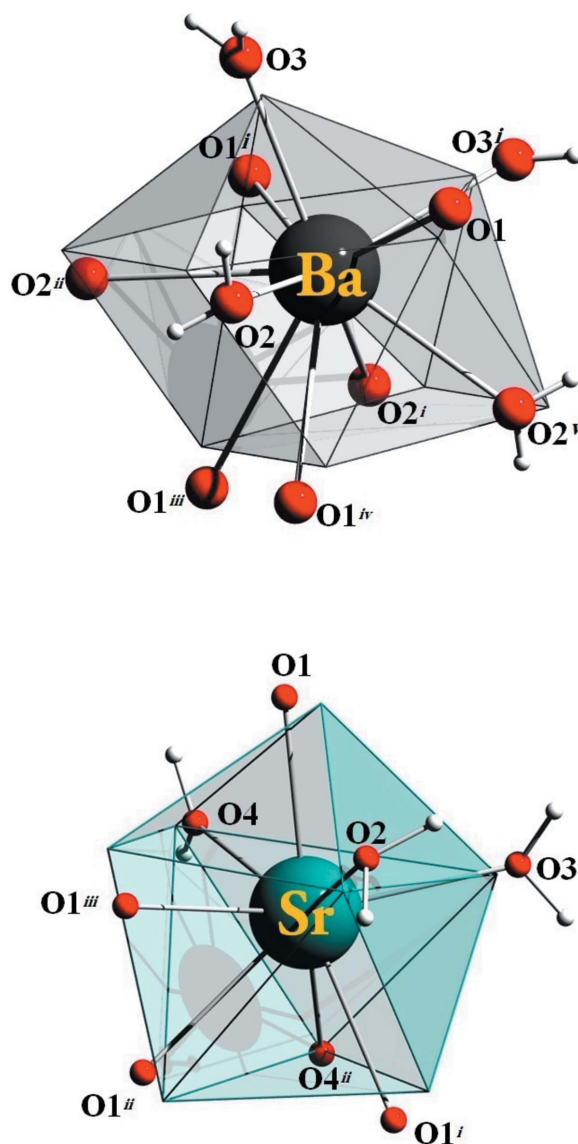
Compound (I) crystallizes in the orthorhombic space group *Imma* while compound (II) crystallizes in *Pmna*. In these two



**Figure 1**  
The coordination environment of the  $Ae^{2+}$  ion in compounds (I) and (II), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes for (I): (i)  $2 - x, \frac{1}{2} - y, z$ ; (ii)  $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} - z$ ; (iii)  $x - \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z$ ; (iv)  $2 - x, y, z$ ; (v)  $\frac{1}{2} + x, y, \frac{1}{2} - z$ ; (vi)  $x - \frac{1}{2}, -y, z$ ; (vii)  $-x - \frac{1}{2}, y, \frac{1}{2} - z$ ; and for (II): (i)  $2 - x, y, z$ ; (ii)  $\frac{1}{2} - x, y, \frac{1}{2} - z$ ; (iii)  $x + \frac{1}{2}, y, \frac{1}{2} - z$ .]

coordination compounds, the asymmetric unit comprises half of a crystallographically independent alkaline-earth metal ion, half of a deprotonated 4-(tetrazol-5-yl)benzoate anion (ttzbenz), and two halves of water molecules in compound (I) and three halves of water molecules in compound (II) (Fig. 1). The bond distances and angles of the ligands are comparable to those found in the literature for similar systems (Zheng *et al.*, 2009; Jiang *et al.*, 2007; Yu *et al.*, 2009).

The crystal structures of compounds (I) and (II) show similar topologies, the main difference being the coordination polyhedron around the metal center. In compound (I), a slightly distorted  $BaO_{10}$  sphenocorona coordination geometry (Casanova *et al.*, 2005) is observed (Fig. 2). The geometry deviates by 4.424 compared to the theoretical model as proposed by *SHAPE 2.1* software (Casanova *et al.*, 2005; see



**Figure 2**  
Coordinating polyhedra of compounds (I) and (II), the colored polyhedra with open front faces represent the ideal polyhedral shape as calculated by *SHAPE 2.1* [Symmetry codes for (I): (i)  $1 - x, \frac{1}{2} - y, z$ ; (ii)  $1 - x, y, z$ ; (iii)  $-\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} - z$ ; (iv)  $\frac{3}{2} - x, y, \frac{1}{2} - z$ ; (v)  $x, \frac{1}{2} - y, z$ ; and for (II): (i)  $2 - x, y, z$ ; (ii)  $\frac{1}{2} - x, y, \frac{1}{2} - z$ ; (iii)  $-\frac{1}{2} + x, y, \frac{1}{2} - z$ .]

**Table 1**  
Selected geometric parameters (Å, °) for (I).

Ba1—O1	2.6598 (17)	Ba1—O2	2.8750 (12)
Ba1—O1 <sup>i</sup>	2.6598 (17)	Ba1—O2 <sup>iii</sup>	2.8750 (12)
Ba1—O3 <sup>i</sup>	2.821 (2)	Ba1—O2 <sup>i</sup>	2.8750 (12)
Ba1—O3	2.821 (2)	Ba1—O1 <sup>ii</sup>	3.0157 (17)
Ba1—O2 <sup>ii</sup>	2.8750 (12)	Ba1—O1 <sup>iii</sup>	3.0157 (17)
O1—Ba1—O1 <sup>i</sup>	137.57 (7)	O2 <sup>ii</sup> —Ba1—O2 <sup>iii</sup>	142.501 (17)
O1—Ba1—O3 <sup>i</sup>	75.09 (3)	O2—Ba1—O2 <sup>iii</sup>	91.23 (5)
O3 <sup>i</sup> —Ba1—O3	89.36 (11)	O1—Ba1—O1 <sup>ii</sup>	132.46 (5)
O1—Ba1—O2 <sup>ii</sup>	134.06 (2)	O3 <sup>i</sup> —Ba1—O1 <sup>ii</sup>	131.51 (5)
O1 <sup>i</sup> —Ba1—O2 <sup>ii</sup>	62.43 (2)	O2 <sup>ii</sup> —Ba1—O1 <sup>ii</sup>	58.35 (2)
O3 <sup>i</sup> —Ba1—O2 <sup>ii</sup>	74.10 (4)	O2—Ba1—O1 <sup>ii</sup>	85.73 (2)
O3—Ba1—O2 <sup>ii</sup>	136.98 (2)	O1 <sup>ii</sup> —Ba1—O1 <sup>iii</sup>	42.49 (6)
O2 <sup>ii</sup> —Ba1—O2	76.81 (4)		

Symmetry codes: (i)  $-x + 1, -y + \frac{3}{2}, z$ ; (ii)  $x, y + \frac{1}{2}, -z + 1$ ; (iii)  $-x + 1, -y + 1, -z + 1$ .

Table S1 in the supporting information). In (I), the barium cation is decacoordinated by four oxygen atoms from three ttzbenz ligands, two independent oxygen atoms from two terminal water molecules (O2 and O3) and four additional oxygens from bridging water molecules. In compound (II), the Sr<sup>2+</sup> ion is eightfold coordinated, being surrounded by four bridging water molecules and by four oxygen atoms from three symmetry-related ttzbenz ligands (Fig. 2), thus generating a triangular dodecahedral SrO<sub>8</sub> coordination geometry; this geometry deviates by 3.426 compared to the theoretical model proposed by *SHAPE 2.1* software (Casanova *et al.*, 2005; see Table S1 in the supporting information).

The bond angles (Tables 1 and 2) around the Ae<sup>2+</sup> ion (Ae<sup>2+</sup> = Ba<sup>2+</sup> and Sr<sup>2+</sup>) range between 42.49 (6) and 142.50 (2)° in compound (I), and between 48.93 (6) and 148.91 (4)° in compound (II). The Ba—O bond lengths are 2.821 (2) and 2.875 (1) Å for the coordinated water molecule, and 2.660 (2) and 3.016 (2) Å for the ttzbenz oxygen atom (Table 2), and these distances are slightly longer than that in an analogous compound (Fu *et al.*, 2010). The Sr—O bond lengths are

**Table 2**  
Selected geometric parameters (Å, °) for (II).

Sr—O1	2.501 (2)	Sr—O1 <sup>i</sup>	2.6602 (14)
Sr—O3	2.522 (2)	Sr—O4	2.6757 (18)
Sr—O2	2.549 (3)		
O1—Sr—O1 <sup>ii</sup>	140.67 (7)	O3—Sr—O1 <sup>iii</sup>	148.91 (4)
O1—Sr—O3	85.19 (4)	O1—Sr—O4	68.20 (5)
O1—Sr—O2	72.67 (4)	O1 <sup>ii</sup> —Sr—O4	147.71 (5)
O3—Sr—O2	103.31 (9)	O3—Sr—O4	83.72 (5)
O1—Sr—O1 <sup>i</sup>	124.21 (4)	O2—Sr—O4	139.50 (4)
O1 <sup>ii</sup> —Sr—O1 <sup>i</sup>	77.42 (5)	O1 <sup>i</sup> —Sr—O4	97.37 (4)
O3—Sr—O1 <sup>i</sup>	148.91 (4)	O1 <sup>iii</sup> —Sr—O4	66.00 (5)
O2—Sr—O1 <sup>i</sup>	95.91 (7)	O1 <sup>iii</sup> —Sr—O4 <sup>i</sup>	97.37 (4)
O1 <sup>ii</sup> —Sr—O1 <sup>iii</sup>	124.21 (5)	O4—Sr—O4 <sup>i</sup>	80.48 (7)

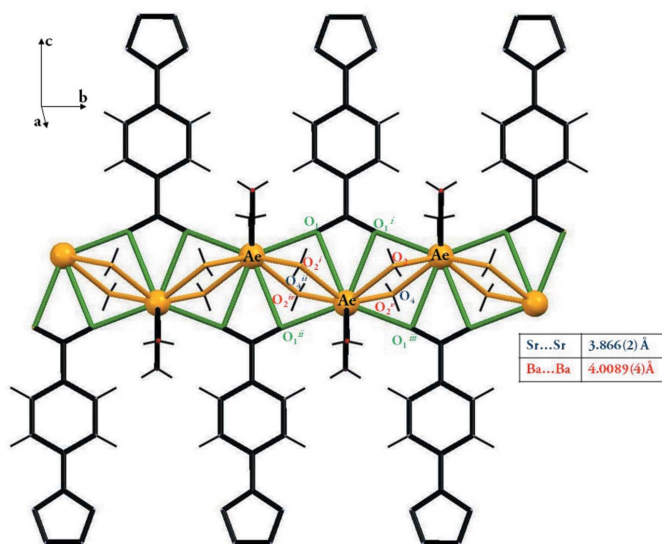
Symmetry codes: (i)  $x - \frac{1}{2}, y, -z + \frac{1}{2}$ ; (ii)  $-x + 1, y, z$ ; (iii)  $-x + \frac{3}{2}, y, -z + \frac{1}{2}$ .

2.501 (2) and 2.660 (1) Å for the ttzbenz oxygen atom, and 2.549 (2) and 2.676 (2) Å for the coordinated water molecule (Table 2). The Ba—O bonds are longer than Sr—O bonds; this is due not only to the nature of the metal, but also, in part, to the measurement temperature [room temperature for compound (I), but 150K for compound (II)]. These bond-length values are close to those observed in similar compounds based on Ae<sup>2+</sup> one-dimensional coordination polymers: Ba—O = 2.647–3.179 Å, Sr—O = 2.486–2.843 Å in [C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>13</sub>Cl<sub>2</sub>CuSr]<sub>n</sub> and [C<sub>24</sub>H<sub>28</sub>N<sub>2</sub>O<sub>13</sub>Cl<sub>2</sub>CuBa]<sub>n</sub> (Hari, *et al.*, 2017), and in the compounds [C<sub>8</sub>H<sub>16</sub>N<sub>16</sub>O<sub>19</sub>Sr<sub>4</sub>]<sub>n</sub> and [C<sub>8</sub>H<sub>20</sub>N<sub>16</sub>O<sub>18</sub>Sr<sub>4</sub>]<sub>n</sub> where the Sr—O distances range from 2.570–2.700 Å and 2.541–2.633 Å, respectively. In the two-dimensional coordination compound [C<sub>2</sub>H<sub>6</sub>Ba<sub>4</sub>N<sub>4</sub>O<sub>5</sub>]<sub>n</sub>, the Ba—O distances are 2.790 and 2.902 Å (Hartdegen *et al.*, 2009), while in the three-dimensional polymers [Ba<sub>2</sub>M(HCOO)<sub>6</sub>(H<sub>2</sub>O)<sub>4</sub>]<sub>n</sub>, Ba—O = 2.801 (2)–3.6143 (2) Å for M = Ni, Ba—O = 2.797 (2)–2.999 (2) Å for M = Zn, and Ba—O = 2.801 (2)–3.004 (2) Å for M = Co (Baggio *et al.*, 2004), and in the strontium complex C<sub>6</sub>H<sub>12</sub>SrN<sub>6</sub>O<sub>10</sub>, Sr—O = 2.506–2.724 Å (Divya *et al.*, 2017).

The ttzbenz ligand can adopt several coordination modes by involving the tetrazole ring (Yao *et al.*, 2013), or the carboxylate group as in our case, where the two compounds use the ttzbenz anion to coordinate two adjacent Ae<sup>2+</sup> cations in a bidentate chelate manner, thus forming a polyatomic bridge and binding neighboring Ae<sup>2+</sup> ions in a zigzag manner, resulting in the formation of binuclear units [Ae—O1—Ae—O1] with a Ba···Ba distance of 4.0089 (4) Å for compound (I) and an Sr···Sr distance of 3.866 (2) Å for compound (II) (Fig. 3).

### 3. Supramolecular features

In compound (I), hydrogen bonds between two coordinated water molecules and two nitrogen atoms of the tetrazole ring of the ttzbenz ligand are observed (Table 3), ensuring cohesion between the tetrazole rings and the inorganic [Ba<sub>2</sub>O<sub>2</sub>]<sub>n</sub> chains. In addition to hydrogen bonds, π-stacking interactions between phenyl rings are observed (Fig. 4) with a centroid-centroid distance of 4.035 (1) Å, which enhance the cohesion of the crystal structure.



**Figure 3**  
Coordinating polymers along the *b* axis.

**Table 3**  
 Hydrogen-bond geometry (Å, °) for (I).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2\cdots N2^{iv}$	0.79 (2)	2.14 (2)	2.927 (2)	175 (3)
$O3-H3\cdots N1^v$	0.79 (3)	2.29 (3)	3.069 (2)	169 (3)

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

**Table 4**  
 Hydrogen-bond geometry (Å, °) for (II).

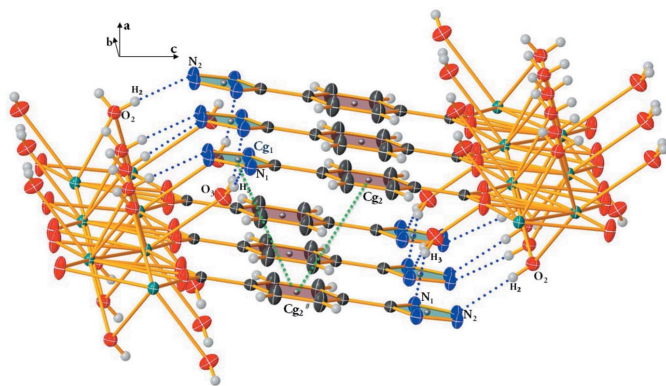
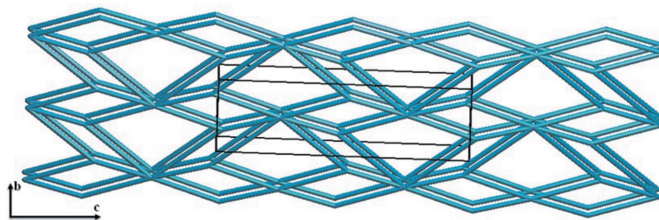
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O3-H3\cdots N1^{iv}$	0.85 (2)	1.96 (2)	2.800 (2)	171 (3)
$O3-H3\cdots N2^{iv}$	0.85 (2)	2.62 (2)	3.314 (3)	141 (2)
$O2-H2\cdots N2^v$	0.77 (3)	2.53 (3)	3.270 (3)	160 (3)
$O4-H4\cdots N2^{vi}$	0.87 (2)	1.93 (2)	2.784 (2)	166 (2)

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

In compound (II), as well as the strong  $O-H\cdots N$  hydrogen bonds (Table 4), weak intramolecular  $\pi$ -stacking interactions are observed, reinforcing the cohesion in the crystal structure between the tetrazole rings (centroid  $Cg1$ ) and the phenyl rings (centroid  $Cg2$ ) with centroid-centroid distances  $Cg1\cdots Cg2 = 3.622$  (3) Å and  $Cg2\cdots Cg2 = 3.897$  (3) Å (Fig. 4).

#### 4. Topological study

To simplify the crystalline structure of the title compounds, we used the standard representation of valence-bound CPs (CP = coordination polymer) to obtain the underlying network. In such models, only metal centers and the centroids of organic ligands are considered as structural units (Alexandrov *et al.*, 2011). The simplification of the crystal structure of the two compounds by this procedure and the topological classification of the two studied compounds led to the same topological network, identified as a 3.6-*c* net with stoichiometry  $(3-C)_2(6-C)$ , which can be represented by the point symbol  $\{4^3\}_2\{4^6.6^6.8^3\}$ . Thus the two structures consist of planar layers running parallel to (100) (Fig. 5).


**Figure 4**  
 Hydrogen bonds (blue dashed lines) and  $\pi$ -stacking interactions (green dashed lines) in the crystal packing of compounds (I) and (II).

**Figure 5**  
 Simplification of the coordination framework in the two compounds using standard representation for valence-bonded CPs.

#### 5. Database survey

A search for 4-(tetrazol-5-yl) benzoate in the Cambridge Structural Database (CSD Version 5.40; Groom *et al.*, 2016) gave 81 hits for the ligand, alone or with co-ligands. The ttzbenz ligand has proved to be an excellent component for the assembly of new coordination complexes and polymers, whether through a bridging and/or chelating coordination mode, mono or polydentate, and as an acceptor of hydrogen bonds through the two carboxylate and tetrazolate groups. This has led to structural diversity with interesting physico-chemical properties, as seen in the structures with metal ions: copper (Ouellette *et al.*, 2009), cobalt (Ouellette *et al.*, 2012), zinc (Wei *et al.*, 2012; Jiang *et al.*, 2007; Zheng *et al.*, 2009), lead (Sun *et al.*, 2013), manganese and cadmium (Cheng *et al.*, 2016; Yu *et al.*, 2009), europium, terbium (Wang *et al.*, 2011). Finally, with bipyridine co-ligands (Yang *et al.*, 2017; Gao *et al.*, 2016), (terpyridinyl)benzoate (Zhang *et al.*, 2016), phenanthroline (Werrett *et al.*, 2015), 3,5-dimethyl-1,2,4-triazolato (Sheng *et al.*, 2016), and *N,N*-dimethylacetamide (Wang *et al.*, 2015).

#### 6. Synthesis and crystallization

Colorless crystals suitable for X-ray diffraction were obtained by hydrothermal synthesis in an aqueous solution according to a literature procedure (Demko & Sharpless, 2001; Zhao *et al.*, 2008), where an aqueous solution (10 ml) of sodium azide (0.065 g, 1 mmol) and 4-cyanobenzoyl chloride (0.165 g, 1 mmol) was added dropwise to an aqueous solution (5 ml) of  $BaCl_2 \cdot 2H_2O$  (0.244 g, 1 mmol) for (I) and  $SrCl_2 \cdot 6H_2O$  (0.266 g, 1 mmol) for (II) under constant stirring for a few minutes. The resulting solution was sealed in a 25 ml teflon-lined stainless steel autoclave and heated at 453 K for 3 d.

The FT-IR spectra for compounds (I) and (II) were recorded in the frequency range  $4000-400\text{ cm}^{-1}$  on a Perkin Elmer FT-IR spectrophotometer Spectrum 1000. The  $\nu$ ,  $\gamma$  and  $\delta$  modes are: stretching, out-of-plane bending, and in-plane bending, respectively. The absence of bands in the two regions:  $2200-2280\text{ cm}^{-1}$  and  $2100-2270\text{ cm}^{-1}$  corresponding to the functions  $-CN$  and  $N_3^-$ , respectively, confirms that the  $[2+3]$  cycloaddition reaction between the cyano group and the azide anions occurred and the tetrazolate ligand was formed (Hammerl *et al.*, 2002, 2003; Damavarapu *et al.*, 2010; Zhang *et al.*, 2013).

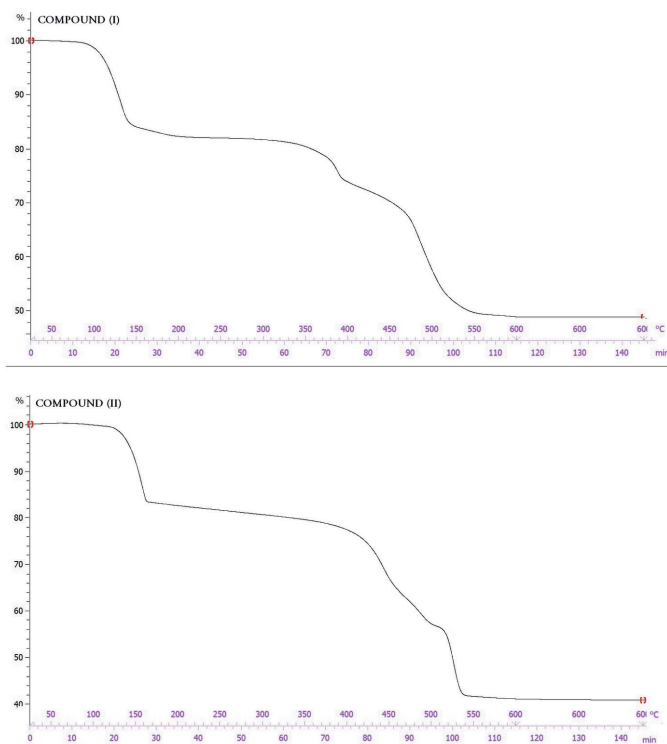
FT-IR of (I) (ATR,  $\text{cm}^{-1}$ ): 3300  $\nu(\text{O}-\text{H})_{\text{water}}$ , 3100  $\nu(\text{C}-\text{H})_{\text{Ph}}$ , 1435  $\nu_{\text{sym}}(\text{C}-\text{C})$ , 1523  $\nu(\text{N}-\text{N})_{\text{ring}}$ , 1603  $\nu(\text{C}-\text{N})_{\text{ring}}$ , 628–1050  $\gamma, \delta$  (tetrazole).

FT-IR of (II) (ATR,  $\text{cm}^{-1}$ ): 3600  $\nu(\text{O}-\text{H})_{\text{water}}$ , 3200  $\nu(\text{C}-\text{H})_{\text{Ph}}$ , 1408  $\nu_{\text{sym}}(\text{C}-\text{C})$ , 1530  $\nu(\text{N}-\text{N})_{\text{ring}}$ , 1585  $\nu(\text{C}-\text{N})_{\text{ring}}$ , 654–1009  $\gamma, \delta$  (tetrazole) (see Fig. S1 in the supporting information).

The thermogravimetric analysis (TGA) was performed in the range 25–600°C under air atmosphere at a flow rate of 5°C/min (Fig. 6). The pyrolytic processes for compound (I) occurs in two main steps. The first step corresponds to the release of four water molecules (2 bridging water molecules and 2 monodentate) (scheme1) between 90°C and 200°C, which corresponds to approximately 18% of the weight of (I). Subsequently, the ligands undergo pyrolysis to result in decomposition (32% by weight) in the range of 200 to 600°C. In compound (II), the pyrolytic processes also go through two stages. The first step corresponds to the release of three water molecules (1 bridging water molecule and 2 monodentate) (scheme1) between 100°C and 160°C, which corresponds to approximately 16% of the weight of (II). The second step corresponding to a weight loss of 44% of (II) is attributed to the decomposition of the ligand between 160 and 600°C.

## 7. Thermogravimetric analysis

The thermogravimetric analysis (TGA) was performed in the range 25–600°C under an air atmosphere at a flow rate of 5°C  $\text{min}^{-1}$  (Fig. 6). The pyrolytic processes for compound (I) occur



**Figure 6**  
Thermogravimetric analysis of compounds (I) and (II).

in two main steps. The first step corresponds to the release of four water molecules (two bridging water molecules and two monodentate) between 90°C and 200°C, which corresponds to approximately 18% of the weight of (I). Subsequently, the ligands undergo pyrolysis to result in decomposition (32% by weight) in the range 200–600°C. In compound (II), the pyrolytic processes also go through two stages. The first step corresponds to the release of three water molecules (one bridging water molecule and two monodentate) between 100°C and 160°C, which corresponds to approximately 16% of the weight of (II). The second step corresponding to a weight loss of 44% of (II) is attributed to the decomposition of the ligand between 160 and 600°C.

## 8. Fluorescence properties

The fluorescence properties of compounds (I) and (II) were determined from the emission spectra at the same excitation wavelength ( $\lambda_{\text{exc}} = 322 \text{ nm}$ ) on an Agilent Cary Eclipse Fluorescence Spectrophotometer at room temperature. Excitation of the two compounds after dissolution in DMSO leads to similar fluorescence emission spectra. The emission maximum of (I) is observed to shift from 368 to 377 nm and from 371 to 378 nm for II (see Fig. S2 in the supporting information), probably corresponding to  $\pi^* \rightarrow \pi$  or  $\pi^* \rightarrow n$  electronic transition of the aromatic ring ttzbenz ligands (Koşar *et al.*, 2012), due to the close resemblance of the emission band of the two compounds. We also note downward absorption values ranging from compound (I) to (II), which may be due to the increase in the atomic number from  $\text{Sr}^{2+}$  to  $\text{Ba}^{2+}$ .

## 9. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 5. The water H atoms were located in a difference-Fourier map and their positions and isotropic displacement parameters were refined. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms ( $\text{C}-\text{H} = 0.93 \text{ \AA}$ ) with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Acknowledgements

We would like to thank S. Maza and the Fluorescence Spectroscopy staff at the National Biotechnology Research Center, Constantine, Algeria.

## Funding information

Funding for this research was provided by: Unité de Recherche de Chimie Moléculaire et Structurale (UR.CHEMS); Direction Générale de la Recherche Scientifique et du Développement Technologique (DGRSDT) Algérie.

**Table 5**  
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	[Ba(C <sub>8</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>4</sub> ]	[Sr(C <sub>8</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub> )(H <sub>2</sub> O) <sub>3</sub> ]
<i>M<sub>r</sub></i>	397.55	329.82
Crystal system, space group	Orthorhombic, <i>Imma</i>	Orthorhombic, <i>Pmna</i>
Temperature (K)	298	150
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.5012 (1), 7.1444 (1), 24.7457 (5)	6.914 (6), 7.018 (7), 24.164 (2)
<i>V</i> (Å <sup>3</sup> )	1326.16 (4)	1172.5 (16)
<i>Z</i>	4	4
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
<i>μ</i> (mm <sup>-1</sup> )	3.02	4.62
Crystal size (mm)	0.6 × 0.5 × 0.22	0.20 × 0.1 × 0.07
Data collection		
Diffractometer	Bruker APEXII CCD	Bruker APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2011)	Multi-scan ( <i>SADABS</i> ; Bruker, 2011)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.670, 0.747	0.67, 0.747
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	5216, 952, 920	9495, 2091, 1740
<i>R<sub>int</sub></i>	0.032	0.038
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.667	0.735
Refinement		
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.016, 0.039, 1.07	0.028, 0.062, 1.07
No. of reflections	937	2091
No. of parameters	70	105
No. of restraints	0	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.91, -0.31	0.65, -0.44

Computer programs: *APEX2* and *SAINT* (Bruker, 2011), *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015a), *SIR92* (Altomare *et al.*, 1993), *SHELXL* (Sheldrick, 2015b), *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

## References

- Alexandrov, E. V., Blatov, V. A., Kochetkov, A. V. & Proserpio, D. M. (2011). *CrystEngComm*, **13**, 3947–3958.
- Altomare, A., Casciarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
- Baggio, R., Stoilova, D., Polla, G., Leyva, G. & Garland, M. T. (2004). *J. Mol. Struct.* **697**, 173–180.
- Bruker (2011). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc, Madison, Wisconsin, USA.
- Casanova, D., Llunell, M., Alemany, P. & Alvarez, S. (2005). *Chem. Eur. J.* **11**, 1479–1494.
- Cheng, M., Ding, Y.-S., Zhang, Z. & Jia, Q.-X. (2016). *Inorg. Chim. Acta*, **450**, 1–7.
- Damavarapu, R., Klapötke, T. M., Stierstorfer, J. & Tarantik, K. R. (2010). *Propellants, Explosives, Pyrotech.* **35**, 395–406.
- Demko, Z. P. & Sharpless, K. B. (2001). *J. Org. Chem.* **66**, 7945–7950.
- Divya, R., Nair, L. P., Bijini, B. R., Nair, C. M. K., Gopakumar, N. & Babu, K. R. (2017). *Physica B*, **526**, 37–44.
- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Fischer, N., Klapötke, T. M., Peters, K., Rusan, M. & Stierstorfer, J. (2011). *Z. Anorg. Allg. Chem.* **637**, 1693–1701.
- Fu, D.-W., Dai, J., Ge, J.-Z., Ye, H.-Y. & Qu, Z.-R. (2010). *Inorg. Chem. Commun.* **13**, 282–285.
- Gao, J.-X., Xiong, J. B., Xu, Q., Tan, Y. H., Liu, Y., Wen, H. R. & Tang, Y. Z. (2016). *Cryst. Growth Des.* **16**, 1559–1564.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Hammerl, A., Holl, G., Kaiser, M., Klapötke, Th. M. & Piotrowski, H. (2003). *Z. Anorg. Allg. Chem.* **629**, 2117–2121.
- Hammerl, A., Holl, G., Klapötke, Th. M., Mayer, P., Nöth, H., Piotrowski, H. & Warchhold, M. (2002). *Eur. J. Inorg. Chem.* pp. 834–845.
- Hari, N., Jana, A. & Mohanta, S. (2017). *Inorg. Chim. Acta*, **467**, 11–20.
- Hartdegen, V., Klapötke, T. M. & Sproll, S. M. (2009). *Inorg. Chem.* **48**, 9549–9556.
- Jiang, T., Zhao, Y.-F. & Zhang, X.-M. (2007). *Inorg. Chem. Commun.* **10**, 1194–1197.
- Klapötke, T. M. & Stierstorfer, J. (2009). *J. Am. Chem. Soc.* **131**, 1122–1134.
- Koşar, B., Albayrak, C., Ersanlı, C. C., Odabaşoğlu, M. & Büyükgüngör, O. (2012). *Spectrochim. Acta A Mol. Biomol. Spectrosc.* **93**, 1–9.
- Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
- Ouellette, W., Darling, K. & Zubieta, J. (2012). *Inorg. Chim. Acta*, **391**, 36–43.
- Ouellette, W., Liu, H., O'Connor, C. J. & Zubieta, J. (2009). *Inorg. Chem.* **48**, 4655–4657.
- Rigaku OD (2015). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Sheng, D.-H., Dan, W.-Y., Luo, G.-X. & Deng, M.-L. (2016). *Chin. J. Struct. Chem.* **35**, 264–270.
- Spek, A. L. (2020). *Acta Cryst.* **E76**, 1–11.
- Sun, J.-Y., Wang, L., Zhang, D.-J., Li, D., Cao, Y., Zhang, L.-Y., Zeng, S.-L., Pang, G.-S., Fan, Y., Xu, J.-N. & Song, T.-Y. (2013). *CrystEngComm*, **15**, 3402–3411.

- Wang, D., Zhang, L., Li, G., Huo, Q. & Liu, Y. (2015). *RSC Adv.* **5**, 18087–18091.
- Wang, J., Nie, J. & Dai, C. (2011). *J. Coord. Chem.* **64**, 1645–1653.
- Wei, Q., Yang, D., Larson, T. E., Kinnibrugh, T. L., Zou, R., Henson, N. J., Timofeeva, T., Xu, H., Zhao, Y. & Mattes, B. R. (2012). *J. Mater. Chem.* **22**, 10166–10171.
- Werrett, M. V., Huff, G. S., Muzzioli, S., Fiorini, V., Zacchini, S., Skelton, B. W., Maggiore, A., Malicka, J. M., Cocchi, M., Gordon, K. C., Stagni, S. & Massi, M. (2015). *Dalton Trans.* **44**, 8379–8393.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
- Yang, H.-Y., Li, Y.-Z., Shi, W.-J., Hou, L., Wang, Y. & Zhu, Z. (2017). *Dalton Trans.* **46**, 11722–11727.
- Yao, R.-X., Qin, Y.-L., Ji, F., Zhao, Y.-F. & Zhang, X.-M. (2013). *Dalton Trans.* **42**, 6611–6618.
- Yu, Z.-P., Xiong, S.-S., Yong, G.-P. & Wang, Z.-Y. (2009). *J. Coord. Chem.* **62**, 242–248.
- Zhang, T., Li, R. F., Tian, A. Q., Feng, X. & Tian, P. H. (2016). *Chin. J. Struct. Chem.* **35**, 1122–1128.
- Zhang, X. B., Ren, Y. H., Li, W., Zhao, F. Q., Yi, J. H., Wang, B. Z. & Song, J. R. (2013). *J. Coord. Chem.* **66**, 2051–2064.
- Zhao, H., Qu, Z.-R., Ye, H.-Y. & Xiong, R.-G. (2008). *Chem. Soc. Rev.* **37**, 84–100.
- Zheng, S.-L., Wang, Y., Yu, Z., Lin, Q. & Coppens, P. (2009). *J. Am. Chem. Soc.* **131**, 18036–18037.

## supporting information

*Acta Cryst.* (2020). E76, 877-883 [https://doi.org/10.1107/S2056989020006386]

***In situ* synthesis, crystal structures, topology and photoluminescent properties of poly[di- $\mu$ -aqua-diaqua[ $\mu_3$ -4-(1*H*-tetrazol-1-*id*-5-yl)benzoato- $\kappa^4$ O:O,O':O'']barium(II)] and poly[ $\mu$ -aqua-diaqua[ $\mu_3$ -4-(1*H*-tetrazol-1-*id*-5-yl)benzoato- $\kappa^4$ O:O,O':O'']strontium(II)]**

**Mohamed Abdellatif Bensegueni, Aouatef Cherouana and Hocine Merazig**

**Computing details**

For both structures, data collection: *APEX2* (Bruker, 2011). Cell refinement: *SAINT* (Bruker, 2011) for (I); *CrysAlis PRO* (Rigaku OD, 2015) for (II). Data reduction: *SAINT* (Bruker, 2011) for (I); *CrysAlis PRO* (Rigaku OD, 2015) for (II). Program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a) for (I); *SIR92* (Altomare *et al.*, 1993) for (II). Program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b) for (I); *SHELXL97* (Sheldrick, 2008) for (II). Molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) for (I); *ORTEP-3 for Windows* (Farrugia, 2012), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2020) for (II). Software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) for (I); *PLATON* (Spek, 2020); *pubCIF* (Westrip, 2010) for (II).

**Poly[di- $\mu$ -aqua-diaqua[ $\mu_3$ -5-(4-carboxylatophenyl)-1*H*-1,2,3,4-tetrazol-1-*ido*- $\kappa^4$ O:O,O':O'']barium(II)] (I)**

*Crystal data*

[Ba(C<sub>8</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>)(H<sub>2</sub>O)<sub>4</sub>]  
*M<sub>r</sub>* = 397.55  
 Orthorhombic, *Imma*  
 Hall symbol: -I 2b 2  
*a* = 7.5012 (1) Å  
*b* = 7.1444 (1) Å  
*c* = 24.7457 (5) Å  
*V* = 1326.16 (4) Å<sup>3</sup>  
*Z* = 4

*F*(000) = 768  
*D<sub>x</sub>* = 1.991 Mg m<sup>-3</sup>  
 Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å  
 Cell parameters from 9092 reflections  
 $\theta$  = 4.3–51.0°  
 $\mu$  = 3.02 mm<sup>-1</sup>  
*T* = 298 K  
 Block, colorless  
 0.6 × 0.5 × 0.22 mm

*Data collection*

Bruker APEXII CCD  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2011)  
*T<sub>min</sub>* = 0.670, *T<sub>max</sub>* = 0.747  
 5216 measured reflections

952 independent reflections  
 920 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.032  
 $\theta_{\max}$  = 28.3°,  $\theta_{\min}$  = 4.9°  
*h* = -10→7  
*k* = -9→7  
*l* = -30→32



Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.016$   
 $wR(F^2) = 0.039$   
 $S = 1.07$   
 937 reflections  
 70 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: mixed  
 H atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0155P)^2 + 1.5691P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.91 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.5000	0.7500	0.462655 (6)	0.02050 (7)
O2	0.7739 (2)	0.5000	0.5000	0.0309 (3)
O1	0.5000	0.4029 (2)	0.42376 (7)	0.0385 (4)
O3	0.2356 (3)	0.7500	0.38160 (10)	0.0458 (5)
N2	0.5000	0.1584 (3)	0.08485 (7)	0.0312 (4)
C1	0.5000	0.2500	0.39934 (11)	0.0197 (5)
N1	0.5000	0.0959 (3)	0.13588 (7)	0.0313 (4)
C2	0.5000	0.2500	0.33851 (11)	0.0221 (5)
C3	0.5000	0.0832 (3)	0.31016 (9)	0.0343 (5)
H3A	0.5000	-0.0298	0.3288	0.041*
C5	0.5000	0.2500	0.22580 (12)	0.0243 (6)
C6	0.5000	0.2500	0.16639 (12)	0.0233 (5)
C4	0.5000	0.0829 (3)	0.25423 (9)	0.0369 (6)
H4	0.5000	-0.0302	0.2356	0.044*
H3	0.175 (4)	0.665 (4)	0.3725 (13)	0.072 (9)*
H2	0.834 (3)	0.464 (4)	0.4761 (9)	0.046 (7)*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.02865 (11)	0.01345 (10)	0.01940 (11)	0.000	0.000	0.000
O2	0.0294 (7)	0.0369 (9)	0.0265 (8)	0.000	0.000	-0.0053 (7)
O1	0.0744 (12)	0.0226 (8)	0.0184 (7)	0.000	0.000	-0.0041 (6)
O3	0.0508 (11)	0.0293 (9)	0.0571 (13)	0.000	-0.0202 (10)	0.000
N2	0.0469 (11)	0.0283 (10)	0.0183 (8)	0.000	0.000	-0.0020 (7)
C1	0.0246 (12)	0.0172 (12)	0.0173 (13)	0.000	0.000	0.000
N1	0.0527 (11)	0.0240 (9)	0.0171 (8)	0.000	0.000	-0.0010 (7)
C2	0.0319 (14)	0.0213 (13)	0.0132 (12)	0.000	0.000	0.000
C3	0.0659 (15)	0.0190 (9)	0.0180 (10)	0.000	0.000	0.0022 (8)

C5	0.0337 (14)	0.0231 (14)	0.0162 (13)	0.000	0.000	0.000
C6	0.0298 (13)	0.0223 (13)	0.0179 (13)	0.000	0.000	0.000
C4	0.0718 (17)	0.0193 (9)	0.0196 (10)	0.000	0.000	-0.0033 (8)

*Geometric parameters (Å, °)*

Ba1—O1	2.6598 (17)	N2—N1	1.339 (3)
Ba1—O1 <sup>i</sup>	2.6598 (17)	C1—O1 <sup>iv</sup>	1.249 (2)
Ba1—O3 <sup>i</sup>	2.821 (2)	C1—C2	1.505 (4)
Ba1—O3	2.821 (2)	N1—C6	1.335 (2)
Ba1—O2 <sup>ii</sup>	2.8750 (12)	C2—C3 <sup>iv</sup>	1.383 (3)
Ba1—O2	2.8750 (12)	C2—C3	1.383 (3)
Ba1—O2 <sup>iii</sup>	2.8750 (12)	C3—C4	1.384 (3)
Ba1—O2 <sup>i</sup>	2.8750 (12)	C3—H3A	0.9300
Ba1—O1 <sup>ii</sup>	3.0157 (17)	C5—C4	1.386 (3)
Ba1—O1 <sup>iii</sup>	3.0157 (17)	C5—C4 <sup>iv</sup>	1.386 (3)
O2—H2	0.78 (2)	C5—C6	1.470 (4)
O1—C1	1.249 (2)	C6—N1 <sup>iv</sup>	1.335 (2)
O3—H3	0.80 (3)	C4—H4	0.9300
N2—N2 <sup>iv</sup>	1.308 (4)		
O1—Ba1—O1 <sup>i</sup>	137.57 (7)	Ba1 <sup>iii</sup> —O2—Ba1	88.77 (5)
O1—Ba1—O3 <sup>i</sup>	75.09 (3)	Ba1 <sup>v</sup> —O2—H2	117 (2)
O1 <sup>i</sup> —Ba1—O3 <sup>i</sup>	75.09 (3)	Ba1 <sup>vi</sup> —O2—H2	117 (2)
O1—Ba1—O3	75.09 (3)	Ba1 <sup>vii</sup> —O2—H2	117 (2)
O1 <sup>i</sup> —Ba1—O3	75.09 (3)	Ba1 <sup>iii</sup> —O2—H2	117 (2)
O3 <sup>i</sup> —Ba1—O3	89.36 (11)	Ba1—O2—H2	111.5 (19)
O1—Ba1—O2 <sup>ii</sup>	134.06 (2)	C1—O1—Ba1	172.27 (16)
O1 <sup>i</sup> —Ba1—O2 <sup>ii</sup>	62.43 (2)	C1—O1—Ba1 <sup>v</sup>	97.70 (14)
O3 <sup>i</sup> —Ba1—O2 <sup>ii</sup>	74.10 (4)	Ba1—O1—Ba1 <sup>v</sup>	90.03 (5)
O3—Ba1—O2 <sup>ii</sup>	136.98 (2)	C1—O1—Ba1 <sup>vii</sup>	97.70 (14)
O1—Ba1—O2	62.43 (2)	Ba1—O1—Ba1 <sup>vii</sup>	90.03 (5)
O1 <sup>i</sup> —Ba1—O2	134.06 (2)	C1—O1—Ba1 <sup>iii</sup>	97.70 (14)
O3 <sup>i</sup> —Ba1—O2	74.10 (4)	Ba1—O1—Ba1 <sup>iii</sup>	90.03 (5)
O3—Ba1—O2	136.98 (2)	C1—O1—Ba1 <sup>vi</sup>	97.70 (14)
O2 <sup>ii</sup> —Ba1—O2	76.81 (4)	Ba1—O1—Ba1 <sup>vi</sup>	90.03 (5)
O1—Ba1—O2 <sup>iii</sup>	62.43 (2)	Ba1—O3—H3	127 (2)
O1 <sup>i</sup> —Ba1—O2 <sup>iii</sup>	134.06 (2)	N2 <sup>iv</sup> —N2—N1	109.49 (12)
O3 <sup>i</sup> —Ba1—O2 <sup>iii</sup>	136.98 (2)	O1—C1—O1 <sup>iv</sup>	122.1 (3)
O3—Ba1—O2 <sup>iii</sup>	74.10 (4)	O1—C1—C2	118.95 (13)
O2 <sup>ii</sup> —Ba1—O2 <sup>iii</sup>	142.501 (17)	O1 <sup>iv</sup> —C1—C2	118.95 (13)
O2—Ba1—O2 <sup>iii</sup>	91.23 (5)	O1—C1—Ba1 <sup>vii</sup>	61.05 (13)
O1—Ba1—O2 <sup>i</sup>	134.06 (2)	O1 <sup>iv</sup> —C1—Ba1 <sup>vii</sup>	61.05 (13)
O1 <sup>i</sup> —Ba1—O2 <sup>i</sup>	62.43 (2)	C2—C1—Ba1 <sup>vii</sup>	180.0
O3 <sup>i</sup> —Ba1—O2 <sup>i</sup>	136.98 (2)	O1—C1—Ba1 <sup>iii</sup>	61.05 (13)
O3—Ba1—O2 <sup>i</sup>	74.10 (4)	O1 <sup>iv</sup> —C1—Ba1 <sup>iii</sup>	61.05 (13)
O2 <sup>ii</sup> —Ba1—O2 <sup>i</sup>	91.23 (5)	C2—C1—Ba1 <sup>iii</sup>	180.0
O2—Ba1—O2 <sup>i</sup>	142.501 (17)	O1—C1—Ba1 <sup>vi</sup>	61.05 (13)

O2 <sup>iii</sup> —Ba1—O2 <sup>i</sup>	76.81 (4)	O1 <sup>iv</sup> —C1—Ba1 <sup>vi</sup>	61.05 (13)
O1—Ba1—O1 <sup>ii</sup>	132.46 (5)	C2—C1—Ba1 <sup>vi</sup>	180.0
O1 <sup>i</sup> —Ba1—O1 <sup>ii</sup>	89.97 (5)	O1—C1—Ba1 <sup>v</sup>	61.05 (13)
O3 <sup>i</sup> —Ba1—O1 <sup>ii</sup>	131.51 (5)	O1 <sup>iv</sup> —C1—Ba1 <sup>v</sup>	61.05 (13)
O3—Ba1—O1 <sup>ii</sup>	131.51 (5)	C2—C1—Ba1 <sup>v</sup>	180.0
O2 <sup>ii</sup> —Ba1—O1 <sup>ii</sup>	58.35 (2)	C6—N1—N2	104.94 (19)
O2—Ba1—O1 <sup>ii</sup>	85.73 (2)	C3 <sup>iv</sup> —C2—C3	119.0 (3)
O2 <sup>iii</sup> —Ba1—O1 <sup>ii</sup>	85.73 (2)	C3 <sup>iv</sup> —C2—C1	120.48 (13)
O2 <sup>i</sup> —Ba1—O1 <sup>ii</sup>	58.35 (2)	C3—C2—C1	120.48 (13)
O1—Ba1—O1 <sup>iii</sup>	89.97 (5)	C2—C3—C4	120.6 (2)
O1 <sup>i</sup> —Ba1—O1 <sup>iii</sup>	132.46 (5)	C2—C3—H3A	119.7
O3 <sup>i</sup> —Ba1—O1 <sup>iii</sup>	131.51 (5)	C4—C3—H3A	119.7
O3—Ba1—O1 <sup>iii</sup>	131.51 (5)	C4—C5—C4 <sup>iv</sup>	119.0 (3)
O2 <sup>ii</sup> —Ba1—O1 <sup>iii</sup>	85.73 (2)	C4—C5—C6	120.50 (14)
O2—Ba1—O1 <sup>iii</sup>	58.35 (2)	C4 <sup>iv</sup> —C5—C6	120.50 (14)
O2 <sup>iii</sup> —Ba1—O1 <sup>iii</sup>	58.35 (2)	N1 <sup>iv</sup> —C6—N1	111.1 (3)
O2 <sup>i</sup> —Ba1—O1 <sup>iii</sup>	85.73 (2)	N1 <sup>iv</sup> —C6—C5	124.44 (13)
O1 <sup>ii</sup> —Ba1—O1 <sup>iii</sup>	42.49 (6)	N1—C6—C5	124.44 (13)
Ba1 <sup>v</sup> —O2—Ba1	88.77 (5)	C3—C4—C5	120.4 (2)
Ba1 <sup>vi</sup> —O2—Ba1	88.77 (5)	C3—C4—H4	119.8
Ba1 <sup>vii</sup> —O2—Ba1	88.77 (5)	C5—C4—H4	119.8
O1—Ba1—O2—Ba1 <sup>v</sup>	-57.76 (3)	O1 <sup>ii</sup> —Ba1—O2—Ba1 <sup>vii</sup>	85.62 (2)
O1 <sup>i</sup> —Ba1—O2—Ba1 <sup>v</sup>	171.44 (5)	O1 <sup>iii</sup> —Ba1—O2—Ba1 <sup>vii</sup>	50.97 (3)
O3 <sup>i</sup> —Ba1—O2—Ba1 <sup>v</sup>	-138.96 (4)	O1—Ba1—O2—Ba1 <sup>iii</sup>	-57.76 (3)
O3—Ba1—O2—Ba1 <sup>v</sup>	-67.75 (7)	O1 <sup>i</sup> —Ba1—O2—Ba1 <sup>iii</sup>	171.44 (5)
O2 <sup>ii</sup> —Ba1—O2—Ba1 <sup>v</sup>	144.096 (12)	O3 <sup>i</sup> —Ba1—O2—Ba1 <sup>iii</sup>	-138.96 (4)
O2 <sup>i</sup> —Ba1—O2—Ba1 <sup>v</sup>	69.71 (4)	O3—Ba1—O2—Ba1 <sup>iii</sup>	-67.75 (7)
O1 <sup>ii</sup> —Ba1—O2—Ba1 <sup>v</sup>	85.62 (2)	O2 <sup>ii</sup> —Ba1—O2—Ba1 <sup>iii</sup>	144.096 (12)
O1 <sup>iii</sup> —Ba1—O2—Ba1 <sup>v</sup>	50.97 (3)	O2 <sup>i</sup> —Ba1—O2—Ba1 <sup>iii</sup>	69.71 (4)
O1—Ba1—O2—Ba1 <sup>vi</sup>	-57.76 (3)	O1 <sup>ii</sup> —Ba1—O2—Ba1 <sup>iii</sup>	85.62 (2)
O1 <sup>i</sup> —Ba1—O2—Ba1 <sup>vi</sup>	171.44 (5)	O1 <sup>iii</sup> —Ba1—O2—Ba1 <sup>iii</sup>	50.97 (3)
O3 <sup>i</sup> —Ba1—O2—Ba1 <sup>vi</sup>	-138.96 (4)	O3 <sup>i</sup> —Ba1—O1—Ba1 <sup>v</sup>	133.31 (5)
O3—Ba1—O2—Ba1 <sup>vi</sup>	-67.75 (7)	O2 <sup>ii</sup> —Ba1—O1—Ba1 <sup>v</sup>	84.02 (4)
O2 <sup>ii</sup> —Ba1—O2—Ba1 <sup>vi</sup>	144.096 (12)	O2—Ba1—O1—Ba1 <sup>v</sup>	53.73 (3)
O2 <sup>i</sup> —Ba1—O2—Ba1 <sup>vi</sup>	69.71 (4)	O3 <sup>i</sup> —Ba1—O1—Ba1 <sup>vii</sup>	133.31 (5)
O1 <sup>ii</sup> —Ba1—O2—Ba1 <sup>vi</sup>	85.62 (2)	O2 <sup>ii</sup> —Ba1—O1—Ba1 <sup>vii</sup>	84.02 (4)
O1 <sup>iii</sup> —Ba1—O2—Ba1 <sup>vi</sup>	50.97 (3)	O2—Ba1—O1—Ba1 <sup>vii</sup>	53.73 (3)
O1—Ba1—O2—Ba1 <sup>vii</sup>	-57.76 (3)	O3 <sup>i</sup> —Ba1—O1—Ba1 <sup>iii</sup>	133.31 (5)
O1 <sup>i</sup> —Ba1—O2—Ba1 <sup>vii</sup>	171.44 (5)	O2 <sup>ii</sup> —Ba1—O1—Ba1 <sup>iii</sup>	84.02 (4)
O3 <sup>i</sup> —Ba1—O2—Ba1 <sup>vii</sup>	-138.96 (4)	O2—Ba1—O1—Ba1 <sup>iii</sup>	53.73 (3)
O3—Ba1—O2—Ba1 <sup>vii</sup>	-67.75 (7)	O3 <sup>i</sup> —Ba1—O1—Ba1 <sup>vi</sup>	133.31 (5)
O2 <sup>ii</sup> —Ba1—O2—Ba1 <sup>vii</sup>	144.096 (12)	O2 <sup>ii</sup> —Ba1—O1—Ba1 <sup>vi</sup>	84.02 (4)
O2 <sup>i</sup> —Ba1—O2—Ba1 <sup>vii</sup>	69.71 (4)	O2—Ba1—O1—Ba1 <sup>vi</sup>	53.73 (3)

Symmetry codes: (i)  $-x+1, -y+3/2, z$ ; (ii)  $x, y+1/2, -z+1$ ; (iii)  $-x+1, -y+1, -z+1$ ; (iv)  $-x+1, -y+1/2, z$ ; (v)  $-x+1, y-1/2, -z+1$ ; (vi)  $x, y-1/2, -z+1$ ; (vii)  $x, -y+1, -z+1$ .

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O2—H2···N2 <sup>viii</sup>	0.79 (2)	2.14 (2)	2.927 (2)	175 (3)
O3—H3···N1 <sup>ix</sup>	0.79 (3)	2.29 (3)	3.069 (2)	169 (3)

Symmetry codes: (viii)  $x+1/2, -y+1/2, -z+1/2$ ; (ix)  $x-1/2, -y+1/2, -z+1/2$ .

Poly[ $\mu$ -aqua-diaqua[ $\mu_3$ -5-(4-carboxylatophenyl)-1*H*-1,2,3,4-tetrazol-1-ido- $\kappa^4$ O:O,O':O']strontium(II)] (II)

Crystal data

[Sr(C<sub>8</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>)(H<sub>2</sub>O)<sub>3</sub>]

$M_r = 329.82$

Orthorhombic, *Pmna*

Hall symbol: -P 2ac 2

$a = 6.914$  (6) Å

$b = 7.018$  (7) Å

$c = 24.164$  (2) Å

$V = 1172.5$  (16) Å<sup>3</sup>

$Z = 4$

$F(000) = 656$

$D_x = 1.874$  Mg m<sup>-3</sup>

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

Cell parameters from 10707 reflections

$\theta = 4.9$ – $34.3^\circ$

$\mu = 4.62$  mm<sup>-1</sup>

$T = 150$  K

Prism, colorless

$0.20 \times 0.1 \times 0.07$  mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2011)

$T_{\min} = 0.67, T_{\max} = 0.747$

9495 measured reflections

2091 independent reflections

1740 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 31.5^\circ, \theta_{\min} = 3.4^\circ$

$h = -10 \rightarrow 8$

$k = -10 \rightarrow 8$

$l = -34 \rightarrow 35$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.028$

$wR(F^2) = 0.062$

$S = 1.07$

2091 reflections

105 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 0.7105P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.65$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.44$  e Å<sup>-3</sup>

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr	0.5000	0.41161 (3)	0.285826 (9)	0.01071 (7)
O4	0.7500	0.6752 (3)	0.2500	0.0148 (4)
O2	0.5000	0.0703 (3)	0.32193 (13)	0.0341 (6)
O3	0.5000	0.6090 (3)	0.37304 (8)	0.0201 (4)

O1	0.84065 (19)	0.3310 (2)	0.31160 (5)	0.0157 (3)
C2	1.0000	0.2947 (3)	0.39842 (10)	0.0112 (5)
N1	1.1596 (2)	0.1898 (2)	0.60389 (6)	0.0155 (3)
C4	0.8268 (3)	0.2547 (3)	0.48414 (7)	0.0166 (4)
H4A	0.7101	0.2459	0.5031	0.020*
C5	1.0000	0.2407 (4)	0.51296 (10)	0.0120 (5)
N2	1.0952 (2)	0.1577 (2)	0.65534 (6)	0.0167 (3)
C6	1.0000	0.2079 (3)	0.57327 (10)	0.0120 (5)
C3	0.8269 (3)	0.2818 (3)	0.42714 (7)	0.0166 (4)
H3A	0.7102	0.2912	0.4082	0.020*
C1	1.0000	0.3206 (4)	0.33702 (10)	0.0113 (5)
H3	0.600 (3)	0.668 (4)	0.3839 (10)	0.037 (7)*
H4	0.709 (4)	0.743 (4)	0.2212 (9)	0.036 (8)*
H2	0.584 (4)	0.014 (5)	0.3353 (12)	0.058 (10)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sr	0.00658 (11)	0.01630 (11)	0.00923 (10)	0.000	0.000	0.00006 (10)
O4	0.0141 (10)	0.0173 (8)	0.0131 (9)	0.000	-0.0015 (7)	0.000
O2	0.0211 (13)	0.0223 (12)	0.0590 (18)	0.000	0.000	0.0144 (12)
O3	0.0102 (10)	0.0302 (11)	0.0200 (10)	0.000	0.000	-0.0087 (9)
O1	0.0088 (6)	0.0258 (7)	0.0124 (6)	0.0014 (6)	-0.0017 (5)	0.0045 (5)
C2	0.0120 (12)	0.0107 (10)	0.0107 (11)	0.000	0.000	0.0017 (9)
N1	0.0144 (8)	0.0215 (8)	0.0106 (7)	-0.0015 (6)	-0.0014 (6)	0.0002 (6)
C4	0.0101 (9)	0.0251 (9)	0.0146 (8)	0.0019 (8)	0.0022 (7)	0.0017 (7)
C5	0.0140 (12)	0.0126 (11)	0.0093 (11)	0.000	0.000	-0.0019 (9)
N2	0.0186 (8)	0.0206 (7)	0.0110 (7)	-0.0015 (7)	-0.0010 (6)	0.0000 (6)
C6	0.0134 (12)	0.0112 (10)	0.0114 (11)	0.000	0.000	-0.0019 (9)
C3	0.0102 (9)	0.0260 (9)	0.0137 (8)	0.0023 (7)	-0.0009 (7)	0.0026 (7)
C1	0.0084 (12)	0.0124 (11)	0.0132 (11)	0.000	0.000	0.0007 (9)

*Geometric parameters (Å, °)*

Sr—O1	2.501 (2)	C2—C3	1.387 (2)
Sr—O1 <sup>i</sup>	2.501 (2)	C2—C1	1.495 (3)
Sr—O3	2.522 (2)	N1—C6	1.335 (2)
Sr—O2	2.549 (3)	N1—N2	1.340 (2)
Sr—O1 <sup>ii</sup>	2.6602 (14)	C4—C5	1.389 (2)
Sr—O1 <sup>iii</sup>	2.6602 (14)	C4—C3	1.390 (2)
Sr—O4	2.6757 (18)	C4—H4A	0.9300
Sr—O4 <sup>ii</sup>	2.6757 (18)	C5—C4 <sup>iv</sup>	1.389 (2)
O4—H4	0.89 (2)	C5—C6	1.475 (3)
O2—H2	0.77 (3)	N2—N2 <sup>iv</sup>	1.316 (4)
O3—H3	0.846 (16)	C6—N1 <sup>iv</sup>	1.335 (2)
O1—C1	1.2635 (19)	C3—H3A	0.9300
C2—C3 <sup>iv</sup>	1.387 (2)	C1—O1 <sup>iv</sup>	1.2635 (19)

O1—Sr—O1 <sup>i</sup>	140.67 (7)	O4 <sup>ii</sup> —Sr—Sr <sup>ii</sup>	43.74 (4)
O1—Sr—O3	85.19 (4)	C1 <sup>ii</sup> —Sr—Sr <sup>ii</sup>	64.037 (19)
O1 <sup>i</sup> —Sr—O3	85.20 (4)	O1—Sr—Sr <sup>v</sup>	43.07 (4)
O1—Sr—O2	72.67 (4)	O1 <sup>i</sup> —Sr—Sr <sup>v</sup>	162.46 (3)
O1 <sup>i</sup> —Sr—O2	72.67 (4)	O3—Sr—Sr <sup>v</sup>	111.97 (2)
O3—Sr—O2	103.31 (9)	O2—Sr—Sr <sup>v</sup>	98.82 (3)
O1—Sr—O1 <sup>ii</sup>	124.21 (4)	O1 <sup>ii</sup> —Sr—Sr <sup>v</sup>	88.51 (4)
O1 <sup>i</sup> —Sr—O1 <sup>ii</sup>	77.42 (5)	O1 <sup>iii</sup> —Sr—Sr <sup>v</sup>	39.95 (3)
O3—Sr—O1 <sup>ii</sup>	148.91 (4)	O4—Sr—Sr <sup>v</sup>	43.74 (4)
O2—Sr—O1 <sup>ii</sup>	95.91 (7)	O4 <sup>ii</sup> —Sr—Sr <sup>v</sup>	115.64 (3)
O1—Sr—O1 <sup>iii</sup>	77.42 (5)	C1 <sup>ii</sup> —Sr—Sr <sup>v</sup>	64.037 (19)
O1 <sup>i</sup> —Sr—O1 <sup>iii</sup>	124.21 (5)	Sr <sup>ii</sup> —Sr—Sr <sup>v</sup>	126.79 (4)
O3—Sr—O1 <sup>iii</sup>	148.91 (4)	Sr—O4—Sr <sup>v</sup>	92.52 (8)
O2—Sr—O1 <sup>iii</sup>	95.91 (7)	Sr—O4—H4	114.6 (18)
O1 <sup>ii</sup> —Sr—O1 <sup>iii</sup>	48.93 (6)	Sr <sup>v</sup> —O4—H4	108.9 (17)
O1—Sr—O4	68.20 (5)	Sr—O2—H2	129 (2)
O1 <sup>i</sup> —Sr—O4	147.71 (5)	Sr—O3—H3	121.9 (18)
O3—Sr—O4	83.72 (5)	C1—O1—Sr	162.79 (14)
O2—Sr—O4	139.50 (4)	C1—O1—Sr <sup>v</sup>	94.66 (12)
O1 <sup>ii</sup> —Sr—O4	97.37 (4)	Sr—O1—Sr <sup>v</sup>	96.98 (5)
O1 <sup>iii</sup> —Sr—O4	66.00 (5)	C3 <sup>iv</sup> —C2—C3	119.4 (2)
O1—Sr—O4 <sup>ii</sup>	147.71 (5)	C3 <sup>iv</sup> —C2—C1	120.32 (11)
O1 <sup>i</sup> —Sr—O4 <sup>ii</sup>	68.20 (5)	C3—C2—C1	120.32 (11)
O3—Sr—O4 <sup>ii</sup>	83.72 (5)	C6—N1—N2	104.81 (16)
O2—Sr—O4 <sup>ii</sup>	139.50 (4)	C5—C4—C3	120.41 (18)
O1 <sup>ii</sup> —Sr—O4 <sup>ii</sup>	66.00 (5)	C5—C4—H4A	119.8
O1 <sup>iii</sup> —Sr—O4 <sup>ii</sup>	97.37 (4)	C3—C4—H4A	119.8
O4—Sr—O4 <sup>ii</sup>	80.48 (7)	C4—C5—C4 <sup>iv</sup>	119.1 (2)
O1—Sr—C1 <sup>ii</sup>	101.29 (3)	C4—C5—C6	120.42 (11)
O1 <sup>i</sup> —Sr—C1 <sup>ii</sup>	101.29 (3)	C4 <sup>iv</sup> —C5—C6	120.42 (11)
O3—Sr—C1 <sup>ii</sup>	158.83 (7)	N2 <sup>iv</sup> —N2—N1	109.42 (10)
O2—Sr—C1 <sup>ii</sup>	97.87 (9)	N1 <sup>iv</sup> —C6—N1	111.5 (2)
O1 <sup>ii</sup> —Sr—C1 <sup>ii</sup>	24.50 (3)	N1 <sup>iv</sup> —C6—C5	124.22 (11)
O1 <sup>iii</sup> —Sr—C1 <sup>ii</sup>	24.50 (3)	N1—C6—C5	124.22 (11)
O4—Sr—C1 <sup>ii</sup>	80.16 (4)	C2—C3—C4	120.34 (18)
O4 <sup>ii</sup> —Sr—C1 <sup>ii</sup>	80.16 (4)	C2—C3—H3A	119.8
O1—Sr—Sr <sup>ii</sup>	162.46 (3)	C4—C3—H3A	119.8
O1 <sup>i</sup> —Sr—Sr <sup>ii</sup>	43.07 (4)	O1—C1—O1 <sup>iv</sup>	121.4 (2)
O3—Sr—Sr <sup>ii</sup>	111.97 (2)	O1—C1—C2	119.31 (11)
O2—Sr—Sr <sup>ii</sup>	98.82 (3)	O1 <sup>iv</sup> —C1—C2	119.31 (11)
O1 <sup>ii</sup> —Sr—Sr <sup>ii</sup>	39.95 (3)	O1—C1—Sr <sup>v</sup>	60.84 (11)
O1 <sup>iii</sup> —Sr—Sr <sup>ii</sup>	88.51 (4)	O1 <sup>iv</sup> —C1—Sr <sup>v</sup>	60.84 (11)
O4—Sr—Sr <sup>ii</sup>	115.64 (3)	C2—C1—Sr <sup>v</sup>	174.84 (17)
O1—Sr—O4—Sr <sup>v</sup>	43.94 (4)	O4 <sup>ii</sup> —Sr—O1—Sr <sup>v</sup>	-59.57 (8)
O1 <sup>i</sup> —Sr—O4—Sr <sup>v</sup>	-158.12 (6)	C1 <sup>ii</sup> —Sr—O1—Sr <sup>v</sup>	29.86 (6)
O3—Sr—O4—Sr <sup>v</sup>	131.27 (4)	Sr <sup>ii</sup> —Sr—O1—Sr <sup>v</sup>	61.70 (12)
O2—Sr—O4—Sr <sup>v</sup>	28.11 (11)	C3—C4—C5—C4 <sup>iv</sup>	0.2 (4)

O1 <sup>ii</sup> —Sr—O4—Sr <sup>v</sup>	-80.03 (4)	C3—C4—C5—C6	-178.7 (2)
O1 <sup>iii</sup> —Sr—O4—Sr <sup>v</sup>	-41.54 (3)	C6—N1—N2—N2 <sup>iv</sup>	-0.35 (16)
O4 <sup>ii</sup> —Sr—O4—Sr <sup>v</sup>	-144.08 (2)	N2—N1—C6—N1 <sup>iv</sup>	0.6 (3)
C1 <sup>ii</sup> —Sr—O4—Sr <sup>v</sup>	-62.52 (4)	N2—N1—C6—C5	-178.6 (2)
Sr <sup>ii</sup> —Sr—O4—Sr <sup>v</sup>	-117.34 (3)	C4—C5—C6—N1 <sup>iv</sup>	-0.1 (4)
O1 <sup>i</sup> —Sr—O1—C1	-74.0 (5)	C4 <sup>iv</sup> —C5—C6—N1 <sup>iv</sup>	-179.0 (2)
O3—Sr—O1—C1	2.4 (5)	C4—C5—C6—N1	179.0 (2)
O2—Sr—O1—C1	-103.1 (5)	C4 <sup>iv</sup> —C5—C6—N1	0.1 (4)
O1 <sup>ii</sup> —Sr—O1—C1	171.6 (5)	C3 <sup>iv</sup> —C2—C3—C4	-0.5 (4)
O1 <sup>iii</sup> —Sr—O1—C1	156.5 (5)	C1—C2—C3—C4	179.0 (2)
O4—Sr—O1—C1	87.6 (5)	C5—C4—C3—C2	0.1 (3)
O4 <sup>ii</sup> —Sr—O1—C1	72.7 (5)	Sr—O1—C1—O1 <sup>iv</sup>	-138.6 (3)
C1 <sup>ii</sup> —Sr—O1—C1	162.1 (5)	Sr <sup>v</sup> —O1—C1—O1 <sup>iv</sup>	-6.2 (3)
Sr <sup>ii</sup> —Sr—O1—C1	-166.1 (4)	Sr—O1—C1—C2	41.6 (6)
Sr <sup>v</sup> —Sr—O1—C1	132.2 (5)	Sr <sup>v</sup> —O1—C1—C2	174.1 (2)
O1 <sup>i</sup> —Sr—O1—Sr <sup>v</sup>	153.83 (6)	Sr—O1—C1—Sr <sup>v</sup>	-132.5 (5)
O3—Sr—O1—Sr <sup>v</sup>	-129.77 (7)	C3 <sup>iv</sup> —C2—C1—O1	179.6 (2)
O2—Sr—O1—Sr <sup>v</sup>	124.67 (8)	C3—C2—C1—O1	0.1 (4)
O1 <sup>ii</sup> —Sr—O1—Sr <sup>v</sup>	39.36 (9)	C3 <sup>iv</sup> —C2—C1—O1 <sup>iv</sup>	-0.1 (4)
O1 <sup>iii</sup> —Sr—O1—Sr <sup>v</sup>	24.29 (6)	C3—C2—C1—O1 <sup>iv</sup>	-179.6 (2)
O4—Sr—O1—Sr <sup>v</sup>	-44.63 (4)		

Symmetry codes: (i)  $-x+1, y, z$ ; (ii)  $x-1/2, y, -z+1/2$ ; (iii)  $-x+3/2, y, -z+1/2$ ; (iv)  $-x+2, y, z$ ; (v)  $x+1/2, y, -z+1/2$ .

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 $\cdots$ N1 <sup>vi</sup>	0.85 (2)	1.96 (2)	2.800 (2)	171 (3)
O3—H3 $\cdots$ N2 <sup>vi</sup>	0.85 (2)	2.62 (2)	3.314 (3)	141 (2)
O2—H2 $\cdots$ N2 <sup>vii</sup>	0.77 (3)	2.53 (3)	3.270 (3)	160 (3)
O4—H4 $\cdots$ N2 <sup>viii</sup>	0.87 (2)	1.93 (2)	2.784 (2)	166 (2)

Symmetry codes: (vi)  $-x+2, -y+1, -z+1$ ; (vii)  $-x+2, -y, -z+1$ ; (viii)  $x-1/2, -y+1, z-1/2$ .