Crystal structure and void analysis of tris(2-amino-1-methylbenzimidazolium) hexakis(nitrato-κ²O,O')lanthanate(III)

Bakhtigul Ruzieva,a,b* Rishad Kunafiev,a,c Zukhra Kadirova,a and Shahlo Daminova,a,b*

*aUzbekistan-Japan Innovation Center of Youth, University street 2B, Tashkent 100095, Uzbekistan, bNational University of Uzbekistan named after Mirzo Ulugbek, University street 4, Tashkent 100174, Uzbekistan, and cState Key Laboratory of Applied Organic Chemistry (SKLAOC), College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, People’s Republic of China. *Correspondence e-mail: b.ruziyeva@nuu.uz, daminova_sh@mail.ru

The organic–inorganic complex salt, \((\text{C}_8\text{H}_{10}\text{N}_3)\text{[La(NO}_3\text{)}_6\text{]}\), comprises a network of N-protonated 2-amino-1-methylbenzimidazolium cations and hexa-kis(nitrato)lanthanate(III) anions. The \(\text{La}^{\text{III}}\) atom is twelve-coordinate within a distorted icosahedral environment. In the unit cell, each pair of the \(\text{La}^{\text{III}}\) atoms lie nearly on one of the crystallographic glide planes. In the crystal structure, there are several N—H···O hydrogen-bonding interactions between the cations and terminal oxygen atoms from the nitrate moieties of the \([\text{La(NO}_3\text{)}_6]\text{]}^{\text{3}–}\) anion. Additional weak C—H···O hydrogen bonds between the cations and anions consolidate the three-dimensional arrangement of the structure. A packing analysis was performed to check the strength of the crystal packing.

1. Chemical context

Layered lanthanide complexes in the solid state or in solution often represent an one-dimensional transition-metal self-assembly (Chen et al., 2017), frequently incorporated within functional groups from various ligand systems. These complexes not only provide excellent opportunities to widen the research scope of rare-earth compounds, but also feature a novel nuclear secondary building unit (SBU), forming porous and intrinsically electrically conductive structures (Skorupskii & Dinca˘, 2020). Although lanthanide ions have characteristic electronic configurations with their complexes being ideal candidates for new crystal structures and potential applications in superconductivity, magnetism, optics, electronics and catalysis (Eliseeva & Bünzli, 2010; Woodruff et al., 2013), lanthanide complexes, especially polynuclear clusters, are not well understood (Barry et al., 2016). Some reasons for this are the uncontrollable polynuclear arrangement of lanthanide complexes and the nature of lanthanide ions, with their high coordination numbers, kinetic instabilities, uncertain preferred stereochemistry, and the variable nature of their coordination spheres.

In this context, originally trying to isolate polynuclear mixed-ligand lanthanum complexes, we have isolated the title organic–inorganic complex lanthanum salt, 3\(\text{C}_8\text{H}_{10}\text{N}_3\text{[La(NO}_3\text{)}_6\text{]}\), tris(2-amino-1-methylbenzimidazolium)hexakis(nitrato-O,O')-lanthanate(III), (I), and report here its crystal structure and void analysis.
2. Structural commentary

The La\textsuperscript{III} atom in (I) (Fig. 1) is twelve-coordinate by O atoms of the nitrato ligands with La—O bond lengths varying between 2.612 (2) and 2.707 (2) Å (Table 1). The nitrato ligands in the resulting [La(NO\textsubscript{3})\textsubscript{6}]\textsuperscript{3–} anion surround the La\textsuperscript{III} atom in a highly distorted icosahedral environment. Bond lengths and angles in the [La(NO\textsubscript{3})\textsubscript{6}]\textsuperscript{3–} anion show no significant deviations from those of other structures where the La\textsuperscript{III} atom is coordinated by nitrate anions and/or water molecules (Drew \textit{et al.}, 1998; Fowkes & Harrison, 2006; Skelton \textit{et al.}, 2019; Polyzou \textit{et al.}, 2012; Bezzubov \textit{et al.}, 2017).

In the unit-cell of (I), each pair of La\textsuperscript{III} atoms nearly lie on each of the crystallographic glide planes [with deviations from the mean planes of 0.00 (7)–0.02 (1) Å]. The intersection between the La\textsuperscript{III} atoms lying on neighboring glide planes at distances of 12.676 and 14.212 Å, respectively, passes through the center of inversion of the unit-cell.

3. Supramolecular features

In the crystal structure of (I) the nitrate groups coordinate bidentately to the La\textsuperscript{III} atom. The corresponding La—O—N—O planes are close to coplanar, \textit{i.e.} deviate slightly from 180°.

As illustrated in Fig. 2, adjacent benzimidazolium molecules stabilize the [La(NO\textsubscript{3})\textsubscript{6}]\textsuperscript{3–} anion by N—H···O interactions (Fig. 1, Table 2). This arrangement is consolidated by slipped \(\pi···\pi\) interactions between neighbouring benzimidazolium cations \([Cg5···Cg7 = 3.4515 (1)\) and \(Cg6···Cg9 = 3.5038 (1) Å\] with slippages of 0.649 and 0.219; \(Cg5\) and \(Cg7\) are the centroids of the C9–C14 and N13/C22/C17/N14/C23 rings, \(Cg6\) and \(Cg9\) are the centroids of the N10/C14–C9/N11/C15 and N13/C22–C17/N14/C23 rings; Fig. 2). In the structure of (I), apart from the N—H···O interactions, there are two weak C—H···O interactions (Table 2) between adjacent

![Figure 1](image1.png)

The molecular structure of the [La(NO\textsubscript{3})\textsubscript{6}]\textsuperscript{3–} anion and surrounding \(\text{C}_{8}\text{H}_{10}\text{N}_{3}\text{H}_{2}\) cations in (I), showing the atom-labeling scheme. Atomic displacement parameters are drawn at the 30% probability level and H atoms are shown at small spheres of arbitrary radius. Hydrogen bonds are shown as blue dotted lines. [Symmetry codes: (i) \(x, -y + \frac{1}{2}, z - \frac{1}{2}\); (ii) \(x - 1, -y + \frac{3}{2}, z - 1/2\)].

![Figure 2](image2.png)

\(\pi···\pi\) stacking in the crystal structure of (I).

![Table 1](image3.png)

| Selected geometric parameters (Å, °). |
|---------------------------------------|
| La1—O1 2.646 (2) La1—O14 2.6551 (19) |
| La1—O2 2.707 (2) La1—O16 2.674 (2) |
| La1—O5 2.661 (2) N7—C6 1.387 (4)   |
| La1—O7 2.699 (2) N7—C7 1.355 (3)   |
| La1—O8 2.6469 (18) N8—C1 1.395 (3) |
| La1—O10 2.6520 (18) N8—C7 1.341 (4) |
| La1—O11 2.631 (2) N8—C8 1.455 (3)   |
| La1—O13 2.612 (2) N9—C7 1.313 (4)   |
| O1—La1—O2 47.45 (6) O11—La1—O10 47.98 (6) |
| O4—La1—O5 47.96 (6) O13—La1—O14 48.26 (6) |
| O8—La1—O7 47.69 (6) O17—La1—O16 47.80 (6) |

![Table 2](image4.png)

| Hydrogen-bond geometry (Å, °). |
|------------------------------|
| D—H···A  D—H  H···A  D···A  D—H···A |
| C21—H21···O17  0.93 2.64 3.530 (5) 161 |
| C24—H24C···O10  0.96 2.52 3.348 (5) 138 |
| N7—H7···O1  0.86 2.01 2.819 (3) 157 |
| N10—H4A···O4  0.86 2.05 2.889 (3) 164 |
| N12—H6A···O6  0.86 2.10 2.944 (3) 165 |
| N13—H7···O7  0.86 2.11 2.920 (4) 156 |
| N15—H9B···O9  0.86 2.14 2.946 (3) 155 |
| N15ii—H9B···O17  0.86 2.32 3.001 (3) 136 |

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

Ruzieva \textit{et al.} \(\text{C}_{8}\text{H}_{10}\text{N}_{3}\text{H}_{2}\)\[La(NO\textsubscript{3})\textsubscript{6}\] Acta Cryst. (2022). E78, 647–651
[La(NO₃)₆]³⁻ anions and C₈H₁₀N₃⁺ cations (Fig. 3). The three-dimensional network of (I) is assembled from all these intermolecular contacts and interactions (Fig. 4).

4. Void analysis

Molecular surfaces can be used to quite accurately define the size and shape of a molecule, and to visualize the space belonging to a molecule in a crystal. To check whether the title compound is densely packed or not, a void-space analysis was performed. Based on isosurfaces of the procrystal electron density and electron-density mapping (Fig. 5), we have used the conventional approach of mapping void space by rolling a probe sphere of variable radius over a fused-sphere representation to locate and visualize the void space in a crystalline material, as well as readily compute surface areas and void volumes (Spackman et al., 2021; Turner et al., 2011). Fig. 6 shows the unit-cell packing for the title complex with a 0.002 a.u. void surface, and a volume of 388.80 Å³ per unit cell. This result indicates that voids occupy 10.7% of the space and, hence, the molecules can be considered as densely packed in the crystal of (I).

5. Database survey

The structure of the molecular [La(NO₃)₆]³⁻ anion was first reported by Drew et al. (1998). A search of the Cambridge...
Structural Database (CSD, version 5.42, update of September 2021; Groom et al., 2016) revealed that there are six other reports of this moiety. One was obtained from the synthesis of a dinuclear NiII/LaIII complex containing the rare-earth metal in separate ions (Polyzou et al., 2012), the second in research into materials with luminescent properties for developing new drugs (Esteban-Parra et al., 2020), the third is a lanthanum/peptide heterometallic complex with interesting optical properties (Bezzubov et al., 2017), the forth was studied during synthesis and theoretical calculations at the DFT level of di-La complexes with a pendant-armed macrocycle (Fernández-Fernández et al., 2006), the fifth is a heteronuclear nitrato lanthanide complex with interesting magnetic properties (Thatipamula et al., 2019), and the sixth is a pyridine imidazolium lanthanum complex (Skelton et al., 2019). The crystal structure of the last compound comprises the anionic unit as ideal [La(NO3)6]3–, i.e. oppositely faced nitrate moieties lie coplanar to the LaIII atom, forming a paddle-wheel-shaped structure. The latter is one of the closely related structures to (1), with the main difference being the number of cations.

6. Synthesis and crystallization

10 ml of an ethanol solution of La(NO3)3·6H2O (216.8 mg, 0.0005 mmol) was stirred at room temperature for 1 h. Then a 10 ml ethanol solution of 2-amino-1-methylbenzimidazole (220.5 mg, 0.0015 mmol) was gradually added dropwise to the stirring mixture over 50 min at 303 K. Immediately after this, the mixture was heated in a reflux condenser at boiling temperature for 30 min. The solution was filtered and allowed to air-dry at room temperature.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All hydrogen atoms were positioned geometrically with C—H = 0.93–0.96 Å and refined using a riding model with Uiso(H) = 1.5 Ueq(C) for methyl groups and 1.2 Ueq(C) for the other groups. Aromatic/amide hydrogen atoms were refined in a similar manner.

Acknowledgements

The authors acknowledge support from the MIRAI FUND (JICA) and technical equipment support provided by the Institute of bioorganic chemistry of Uzbek Academy of Sciences.

Funding information

Funding for this research was provided by: Japan International Cooperation Agency.

Table 3

| Crystal data | Chemical formula | $(\text{C}_7\text{H}_{10}\text{N}_3)_3[\text{La(NO}_3]_6$ |
|--------------|------------------|---------------------------------------------------|
| $M_r$ | 955.54 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 293 |
| $a$, $b$, $c$ (Å) | 11.78754 (10), 17.59536 (14), 17.79338 (15) |
| $\beta$ (°) | 99.4928 (8) |
| $V$ (Å³) | 3639.92 (5) |
| $Z$ | 4 |
| Radiation type | Cu $K\alpha$ |
| $\mu$ (mm⁻¹) | 9.95 |
| Crystal size (mm) | 0.21 × 0.18 × 0.12 |

| Data collection | Diffractometer |
|-----------------|----------------|
| XtaLAB Synergy, Single source at home/near, HyPix3000 |
| Absorption correction | Multi-scan (CrysAlis PRO; Rigaku OD, 2020) |

| $T_{min}$, $T_{max}$ | 0.281, 1.000 |
| No. of measured, independent and observed $|F| > 2\sigma(F)$ | 21842, 7018, 6305 |
| $R_{int}$ | 0.038 |
| $\sin \theta \lambda_{max}$ (Å⁻¹) | 0.515 |

| Refinement | |
| $R[F^2 > 2\sigma(F)]$, $wR(F^2)$, $S$ | 0.032, 0.089, 1.05 |
| No. of reflections | 7018 |
| No. of parameters | 527 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta \rho_{max}$, $\Delta \rho_{min}$ (e Å⁻³) | 0.69, −0.73 |

Computer programs: CrysAlis PRO (Rigaku OD, 2020), SHELXS (Sheldrick, 2008), SHELXL (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae et al., 2020), OLEX2 (Dolomanov et al., 2009), PLATON (Spek, 2020) and publCIF (Westrip, 2010).
References

Fernández-Fernández, M. del C., Bastida, R., Macias, A., Pérez-Lourido, P., Platas-Iglesias, C. & Valencia, L. (2006). Inorg. Chem. **45**, 4484–4496.

Barry, D. E., Caffrey, D. F. & Gunnlaugsson, T. (2016). Chem. Soc. Rev. **45**, 3244–3274.

Bezzubov, S. I., Bilyalova, A. A., Zharinova, I. S., Lavrova, M. A., Kiselev, Y. M. & Dolzhenko, V. D. (2017). Russ. J. Inorg. Chem. **62**, 1197–1201.

Chen, W., Tang, X., Dou, W., Wang, B., Guo, L., Ju, Z. & Liu, W. (2017). Chem. Eur. J. **23**, 9804–9811.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). J. Appl. Cryst. **42**, 339–341.

Drew, M. G. B., Hudson, M. J., Iveson, P. B., Russell, M. L., Liljenzin, J.-O., Skilberg, M., Spjuth, L. & Madic, C. (1998). J. Chem. Soc. Dalton Trans. pp. 2973–2980.

Eliseeva, S. V. & BüNZli, J. G. (2010). Chem. Soc. Rev. **39**, 189–227.

Esteban-Parra, G. M., Moscoso, I., Cepeda, J., García, J. A., Sánchez-Moreno, M., Rodríguez-Díéguez, A. & Quiroés, M. (2020). Eur. J. Inorg. Chem. pp. 308–317.

Farrugia, L. J. (2012). J. Appl. Cryst. **45**, 849–854.

Fowkes, A. & Harrison, W. T. A. (2006). Acta Cryst. E62, m1301–m1303.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). Acta Cryst. B**72**, 171–179.

Macrae, C. F., Sovago, L., 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.

Polyzou, C. D., Nikolau, H., Papatriantafyllopoulou, C., Psycharis, V., Terzis, A., Raptopoulou, C. P., Escuer, A. & Perlepes, S. P. (2012). Dalton Trans. **41**, 13755–13764.

Rigaku OD (2020). CrysAlis PRO. Rigaku Oxford Diffraction, Yarnton, England.

Sheldrick, G. M. (2008). Acta Cryst. A**64**, 112–122.

Sheldrick, G. M. (2015). Acta Cryst. C**71**, 3–8.

Skelton, B. W., Kokozay, V. N., Vassilyeva, O. Yu. & Buvaylo, E. A. (2019). Private communication (refcode: GOWVIA). CCDC, Cambridge, England.

Skorupskiū, G. & Dincă, M. (2020). J. Am. Chem. Soc. **142**, 6920–6924.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). J. Appl. Cryst. **54**, 1006–1011.

Spek, A. L. (2020). Acta Cryst. E**76**, 1–11.

Thatipamula, K. C., Bhargavi, G. & Rajasekharan, M. V. (2019). Chem. Sel. **4**, 3450–3458.

Turner, M. J., McKinnon, J. J., Jayatilaka, D. & Spackman, M. A. (2011). CrystEngComm. **13**, 1804–1813.

Westrip, S. P. (2010). J. Appl. Cryst. **43**, 920–925.

Woodruff, D. N., Winpenny, R. E. & Layfield, R. A. (2013). Chem. Rev. **113**, 5110–5148.
Crystal structure and void analysis of tris(2-amino-1-methylbenzimidazolium) hexakis(nitrato-κ²O,O')lanthanate(III)

Bakhtigul Ruzieva, Rishad Kunafiev, Zukhra Kadirova and Shahlo Daminova

Computing details

Data collection: CrysAlis PRO (Rigaku OD, 2020); cell refinement: CrysAlis PRO (Rigaku OD, 2020); data reduction: CrysAlis PRO (Rigaku OD, 2020); program(s) used to solve structure: SHELXS (Sheldrick, 2008); program(s) used to refine structure: SHELXL (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012), Mercury (Macrae et al., 2020); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009), PLATON (Spek, 2020), publCIF (Westrip, 2010).

Tris(2-amino-1-methylbenzimidazolium) hexakis(nitrato-κ²O,O')lanthanate(III)

Crystal data

\((\text{C}_8\text{H}_{10}\text{N}_3)\text{[La(NO}_3\text{)_6]}\)

\(M_r = 955.54\)

Monoclinic, \(P2_1/c\)

\(a = 11.78754\) (10) Å

\(b = 17.59536\) (14) Å

\(c = 17.79338\) (15) Å

\(β = 99.4928\) (8)°

\(V = 3639.92\) (5) Å³

\(Z = 4\)

\(F(000) = 1920\)

\(D_x = 1.744\) Mg m⁻³

\(\text{Cu}\ \text{Kα radiation, } λ = 1.54184\ \text{Å}\)

Cell parameters from 13771 reflections

\(θ = 2.5–71.2°\)

\(μ = 9.95\) mm⁻¹

\(T = 293\) K

Block, yellow

\(0.21 \times 0.18 \times 0.12\) mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2020)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R(F^2 > 2σ(F^2)) = 0.032\)

\(wR(F^2) = 0.089\)

\(S = 1.05\)

7018 reflections

527 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\(w = 1/[σ^2(F^2) + (0.054P)^2]\)

where \(P = (F^2 + 2F^2)/3\)

\((Δ/σ)_{\text{max}} = 0.002\)
Δρ_{max} = 0.69 \text{ e Å}^{-3}
Δρ_{min} = -0.73 \text{ e Å}^{-3}

Extinction correction: SHELXL (Sheldrick, 2015a), Fc^2=kFc[1+0.001xFc^2λ^3/sin(2θ)]^{-1/4}
Extinction coefficient: 0.00063 (4)

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 (Å²)

|    | x     | y     | z     | Uiso/Ur |    |
|----|-------|-------|-------|---------|----|
| La1| 0.29343 (2) | 0.24596 (2) | 0.26399 (2) | 0.03257 (8) |    |
| O1 | 0.13909 (18) | 0.35278 (13) | 0.21917 (11) | 0.0522 (5) |    |
| O2 | 0.16522 (19) | 0.33582 (13) | 0.34071 (11) | 0.0586 (5) |    |
| O3 | 0.0273 (2) | 0.40812 (16) | 0.28696 (17) | 0.0880 (9) |    |
| O4 | 0.39500 (18) | 0.38018 (12) | 0.28782 (11) | 0.0498 (5) |    |
| O5 | 0.35777 (17) | 0.34828 (12) | 0.16921 (10) | 0.0482 (5) |    |
| O6 | 0.4493 (2) | 0.45295 (14) | 0.20134 (14) | 0.0794 (7) |    |
| O7 | 0.4095 (2) | 0.25349 (10) | 0.40779 (14) | 0.0475 (6) |    |
| O8 | 0.25431 (15) | 0.18594 (12) | 0.39370 (10) | 0.0487 (5) |    |
| O9 | 0.37164 (18) | 0.18384 (14) | 0.50096 (11) | 0.0627 (6) |    |
| O10| 0.07926 (15) | 0.19647 (12) | 0.25603 (11) | 0.0484 (5) |    |
| O11| 0.20210 (16) | 0.10968 (12) | 0.24177 (11) | 0.0483 (5) |    |
| O12| 0.0197 (2) | 0.08323 (15) | 0.22181 (14) | 0.0737 (7) |    |
| O13| 0.19323 (18) | 0.22778 (13) | 0.12292 (12) | 0.0480 (5) |    |
| O14| 0.36267 (16) | 0.17855 (13) | 0.14595 (11) | 0.0530 (5) |    |
| O15| 0.2596 (2) | 0.16638 (15) | 0.03340 (11) | 0.0679 (6) |    |
| O16| 0.44669 (18) | 0.13478 (12) | 0.30224 (12) | 0.0528 (5) |    |
| O17| 0.52066 (19) | 0.24035 (11) | 0.27129 (13) | 0.0468 (5) |    |
| O18| 0.62845 (18) | 0.14095 (15) | 0.29585 (13) | 0.0683 (6) |    |
| N1 | 0.1087 (2) | 0.36713 (14) | 0.28342 (15) | 0.0511 (6) |    |
| N2 | 0.40091 (19) | 0.39556 (13) | 0.21858 (13) | 0.0460 (5) |    |
| N3 | 0.34526 (18) | 0.20720 (15) | 0.43578 (12) | 0.0435 (5) |    |
| N4 | 0.0971 (2) | 0.12845 (15) | 0.23923 (13) | 0.0453 (6) |    |
| N5 | 0.27197 (19) | 0.18996 (14) | 0.09850 (12) | 0.0426 (5) |    |
| N6 | 0.53406 (19) | 0.17059 (14) | 0.29008 (12) | 0.0449 (5) |    |
| N7 | −0.0092 (2) | 0.40624 (14) | 0.08932 (13) | 0.0515 (6) |    |
| H1 | 0.029959 | 0.401296 | 0.134312 | 0.062* |    |
| N8 | −0.0554 (2) | 0.40492 (13) | −0.03455 (13) | 0.0477 (5) |    |
| N9 | 0.1321 (2) | 0.36555 (16) | 0.01938 (17) | 0.0666 (8) |    |
| H3A| 0.181714 | 0.358860 | 0.060033 | 0.080* |    |
| H3B| 0.150431 | 0.356204 | −0.024523 | 0.080* |    |
| C1 | −0.1515 (2) | 0.43169 (16) | −0.00624 (16) | 0.0457 (6) |    |
| C2 | −0.2576 (3) | 0.4554 (2) | −0.0427 (2) | 0.0644 (9) |    |
| H2 | −0.277566 | 0.454118 | −0.095461 | 0.077* |    |
| C3 | −0.3333 (3) | 0.4813 (3) | 0.0036 (3) | 0.0831 (13) |    |
| H3 | −0.405826 | 0.498305 | −0.018592 | 0.100* |    |
|   | x      | y      | z      | U_{eq}  |
|---|--------|--------|--------|---------|
| C4 | -0.3035 (3) | 0.4826 (3) | 0.0817 (3) | 0.0828 (12) |
| H4 | -0.356791 | 0.500237 | 0.110746 | 0.099* |
| C5 | -0.1968 (3) | 0.4584 (2) | 0.1188 (2) | 0.0645 (9) |
| H5 | -0.177024 | 0.459587 | 0.171542 | 0.077* |
| C6 | -0.1216 (2) | 0.43237 (16) | 0.07252 (16) | 0.0458 (6) |
| C7 | 0.0283 (3) | 0.39002 (16) | 0.02434 (16) | 0.0485 (7) |
| C8 | -0.0481 (3) | 0.3937 (2) | -0.11461 (17) | 0.0681 (10) |
| C9 | -0.123423 | 0.383637 | -0.142553 | 0.102* |
| H8C | 0.001541 | 0.351474 | -0.119738 | 0.102* |
| C10 | 0.7675 (3) | 0.4709 (2) | 0.50060 (18) | 0.0475 (7) |
| H10 | 0.840999 | 0.491168 | 0.588073 | 0.073* |
| C11 | 0.7050 (4) | 0.4467 (2) | 0.62983 (19) | 0.0703 (10) |
| H11 | 0.736881 | 0.451331 | 0.681041 | 0.084* |
| C12 | 0.5960 (3) | 0.4157 (2) | 0.6103 (2) | 0.0671 (9) |
| H12 | 0.556988 | 0.399753 | 0.648861 | 0.081* |
| C13 | 0.5436 (3) | 0.40784 (18) | 0.53563 (19) | 0.0566 (7) |
| H13 | 0.470361 | 0.387121 | 0.522711 | 0.068* |
| C14 | 0.6059 (2) | 0.43245 (16) | 0.48098 (16) | 0.0446 (6) |
| C15 | 0.6674 (2) | 0.46703 (16) | 0.37422 (16) | 0.0466 (6) |
| C16 | 0.8664 (3) | 0.5101 (2) | 0.4250 (2) | 0.0626 (8) |
| H16B | 0.922846 | 0.475477 | 0.450741 | 0.094* |
| H16C | 0.878371 | 0.559568 | 0.447659 | 0.094* |
| N13 | 0.6355 (2) | 0.23763 (14) | 0.50237 (16) | 0.0445 (6) |
| H7 | 0.572120 | 0.228425 | 0.472247 | 0.053* |
| N14 | 0.7613 (2) | 0.24800 (12) | 0.60674 (17) | 0.0454 (6) |
| N15 | 0.5738 (2) | 0.21128 (17) | 0.61913 (15) | 0.0601 (7) |
| H9A | 0.591261 | 0.208013 | 0.667896 | 0.072* |
| H9B | 0.504897 | 0.201377 | 0.596973 | 0.072* |
| C17 | 0.8178 (3) | 0.26746 (17) | 0.54597 (19) | 0.0428 (6) |
| C18 | 0.9309 (2) | 0.28901 (19) | 0.54492 (19) | 0.0532 (7) |
| H18 | 0.985120 | 0.291954 | 0.589167 | 0.064* |
| C19 | 0.9581 (3) | 0.30592 (19) | 0.4736 (2) | 0.0596 (8) |
| H19 | 1.032729 | 0.320673 | 0.469900 | 0.071* |
| C20 | 0.8769 (3) | 0.30138 (19) | 0.40783 (19) | 0.0573 (8) |
| H20 | 0.898241 | 0.313790 | 0.361311 | 0.069* |
| C21 | 0.7647 (3) | 0.2788 (2) | 0.40965 (18) | 0.0520 (7) |
| H21 | 0.710398 | 0.275564 | 0.365475 | 0.062* |
| C22 | 0.7376 (3) | 0.26148 (15) | 0.4800 (2) | 0.0423 (7) |
| C23 | 0.6521 (3) | 0.23136 (18) | 0.57861 (18) | 0.0447 (6) |
|        | U₁¹   | U₂²   | U₃³   | U¹²   | U¹³   | U²³   |
|--------|-------|-------|-------|-------|-------|-------|
| La1    | 0.02761 (11) | 0.04264 (11) | 0.02672 (11) | −0.00091 (5) | 0.00235 (7) | −0.00063 (5) |
| O1     | 0.0533 (12) | 0.0610 (13) | 0.0427 (11) | 0.0138 (10) | 0.0095 (9) | 0.0013 (9) |
| O2     | 0.0657 (13) | 0.0691 (14) | 0.0419 (11) | 0.0064 (11) | 0.0119 (10) | −0.0032 (10) |
| O3     | 0.0832 (18) | 0.0851 (19) | 0.103 (2) | 0.0438 (15) | 0.0375 (16) | 0.0091 (16) |
| O4     | 0.0563 (12) | 0.0531 (12) | 0.0378 (10) | −0.0101 (10) | 0.0015 (9) | −0.0034 (9) |
| O5     | 0.0492 (11) | 0.0588 (12) | 0.0360 (10) | −0.0085 (10) | 0.0051 (8) | −0.0045 (9) |
| O6     | 0.0942 (18) | 0.0657 (15) | 0.0731 (16) | −0.0359 (14) | −0.0013 (13) | 0.0180 (12) |
| O7     | 0.0387 (12) | 0.0676 (15) | 0.0356 (12) | −0.0118 (8) | 0.0045 (9) | 0.0017 (8) |
| O8     | 0.0391 (10) | 0.0704 (14) | 0.0345 (9) | −0.0124 (9) | −0.0006 (8) | 0.0021 (9) |
| O9     | 0.0600 (12) | 0.0911 (17) | 0.0328 (10) | −0.0130 (12) | −0.0048 (9) | 0.0158 (10) |
| O10    | 0.0362 (10) | 0.0572 (13) | 0.0513 (11) | −0.0035 (9) | 0.0059 (8) | −0.0069 (9) |
| O11    | 0.0439 (11) | 0.0488 (12) | 0.0517 (12) | −0.0018 (8) | 0.0064 (9) | −0.0041 (8) |
| O12    | 0.0621 (14) | 0.0842 (18) | 0.0775 (16) | −0.0371 (13) | 0.0193 (12) | −0.0255 (14) |
| O13    | 0.0387 (11) | 0.0629 (12) | 0.0410 (11) | 0.0030 (10) | 0.0027 (9) | −0.0057 (10) |
| O14    | 0.0379 (10) | 0.0772 (15) | 0.0426 (11) | 0.0085 (10) | 0.0027 (8) | −0.0074 (10) |
| O15    | 0.0750 (14) | 0.0911 (18) | 0.0375 (11) | −0.0059 (13) | 0.0091 (10) | −0.0185 (11) |
| O16    | 0.0480 (12) | 0.0536 (12) | 0.0560 (12) | 0.0014 (10) | 0.0067 (9) | 0.0066 (10) |
| O17    | 0.0366 (11) | 0.0610 (13) | 0.0425 (12) | 0.0019 (8) | 0.0053 (9) | 0.0045 (8) |
| O18    | 0.0436 (11) | 0.0835 (17) | 0.0754 (15) | 0.0232 (11) | 0.0027 (10) | −0.0033 (13) |
| N1     | 0.0535 (15) | 0.0479 (14) | 0.0550 (15) | 0.0062 (12) | 0.0182 (12) | −0.0045 (11) |
| N2     | 0.0436 (12) | 0.0445 (13) | 0.0481 (13) | −0.0035 (10) | 0.0023 (10) | 0.0034 (10) |
| N3     | 0.0361 (11) | 0.0619 (15) | 0.0319 (11) | −0.0024 (11) | 0.0041 (9) | 0.0000 (10) |
| N4     | 0.0435 (13) | 0.0570 (15) | 0.0357 (12) | −0.0119 (11) | 0.0073 (10) | −0.0055 (10) |
| N5     | 0.0425 (12) | 0.0542 (14) | 0.0312 (11) | −0.0076 (11) | 0.0062 (9) | −0.0023 (9) |
| N6     | 0.0398 (12) | 0.0600 (15) | 0.0330 (11) | 0.0067 (11) | 0.0006 (9) | −0.0030 (10) |
| N7     | 0.0584 (14) | 0.0567 (15) | 0.0389 (12) | 0.0078 (12) | 0.0070 (11) | 0.0049 (11) |
| N8     | 0.0585 (14) | 0.0471 (13) | 0.0398 (12) | 0.0029 (11) | 0.0149 (11) | −0.0002 (10) |
| N9     | 0.0623 (17) | 0.0686 (18) | 0.0737 (19) | 0.0211 (14) | 0.0248 (14) | 0.0147 (15) |
| C1     | 0.0516 (16) | 0.0414 (15) | 0.0452 (15) | −0.0024 (12) | 0.0106 (12) | −0.0032 (12) |
| C2     | 0.0538 (19) | 0.075 (2) | 0.062 (2) | −0.0026 (17) | 0.0007 (16) | −0.0021 (18) |
| C3     | 0.045 (2) | 0.097 (3) | 0.108 (4) | 0.010 (2) | 0.013 (2) | 0.002 (3) |
| C4     | 0.067 (2) | 0.092 (3) | 0.100 (3) | 0.008 (2) | 0.044 (2) | −0.003 (3) |
| C5     | 0.069 (2) | 0.073 (2) | 0.058 (2) | 0.0051 (18) | 0.0309 (17) | −0.0028 (17) |
| C6     | 0.0511 (16) | 0.0450 (15) | 0.0433 (15) | 0.0008 (13) | 0.0140 (12) | −0.0002 (12) |
| C7     | 0.0549 (17) | 0.0433 (15) | 0.0511 (16) | 0.0071 (13) | 0.0197 (14) | 0.0069 (12) |
| C8     | 0.099 (3) | 0.066 (2) | 0.0451 (17) | −0.0033 (19) | 0.0292 (18) | −0.0037 (15) |
| C9     | 0.0527 (18) | 0.0402 (15) | 0.0479 (16) | 0.0006 (13) | 0.0035 (13) | 0.0018 (12) |
| Atoms | Uiso1 | Uiso2 | Uiso3 | U12 | U13 | U23 |
|-------|-------|-------|-------|-----|-----|-----|
| C10   | 0.064 (2) | 0.063 (2) | 0.0524 (18) | -0.0001 (17) | -0.0026 (15) | -0.0013 (15) |
| C11   | 0.097 (3) | 0.066 (2) | 0.0459 (18) | 0.004 (2) | 0.0034 (18) | 0.0006 (16) |
| C12   | 0.083 (2) | 0.061 (2) | 0.062 (2) | 0.0085 (19) | 0.0247 (19) | 0.0075 (16) |
| C13   | 0.0537 (17) | 0.0481 (17) | 0.070 (2) | 0.0031 (14) | 0.0154 (15) | 0.0049 (15) |
| C14   | 0.0499 (15) | 0.0374 (14) | 0.0521 (16) | 0.0049 (12) | 0.0059 (13) | -0.0008 (12) |
| C15   | 0.0487 (15) | 0.0430 (15) | 0.0453 (15) | -0.0034 (12) | -0.0020 (12) | -0.0022 (12) |
| C16   | 0.0466 (16) | 0.070 (2) | 0.068 (2) | -0.0130 (16) | 0.0000 (14) | 0.0074 (17) |
| N13   | 0.0280 (12) | 0.0551 (14) | 0.0482 (15) | -0.0019 (10) | -0.0003 (11) | -0.0078 (11) |
| N14   | 0.0320 (13) | 0.0571 (17) | 0.0457 (15) | -0.0002 (9) | 0.0028 (12) | -0.0058 (9) |
| N15   | 0.0407 (13) | 0.087 (2) | 0.0537 (15) | -0.0050 (14) | 0.0110 (11) | -0.0069 (15) |
| C17   | 0.0326 (14) | 0.0438 (14) | 0.0507 (17) | 0.0036 (12) | 0.0032 (12) | -0.0056 (13) |
| C18   | 0.0317 (14) | 0.060 (2) | 0.0656 (19) | -0.0028 (13) | 0.0024 (13) | -0.0112 (15) |
| C19   | 0.0440 (16) | 0.061 (2) | 0.076 (2) | -0.0082 (15) | 0.0188 (16) | -0.0096 (17) |
| C20   | 0.0565 (18) | 0.060 (2) | 0.0582 (19) | -0.0075 (15) | 0.0197 (15) | -0.0042 (15) |
| C21   | 0.0505 (17) | 0.0574 (18) | 0.0468 (17) | -0.0019 (15) | 0.0038 (13) | -0.0063 (14) |
| C22   | 0.0318 (14) | 0.0418 (15) | 0.0535 (19) | 0.0018 (11) | 0.0073 (13) | -0.0078 (12) |
| C23   | 0.0335 (15) | 0.0509 (15) | 0.0484 (17) | 0.0051 (13) | 0.0032 (12) | -0.0047 (13) |
| C24   | 0.051 (2) | 0.095 (3) | 0.049 (2) | -0.0038 (16) | -0.0054 (17) | -0.0030 (15) |

**Geometric parameters (Å, °)**

| Bond/Distance | Length/Distance (Å) | Angle (°) |
|---------------|---------------------|-----------|
| La1—O1       | 2.646 (2)           |           |
| La1—O2       | 2.707 (2)           |           |
| La1—O4       | 2.650 (2)           |           |
| La1—O5       | 2.661 (2)           |           |
| La1—O7       | 2.699 (2)           |           |
| La1—O8       | 2.6469 (18)         |           |
| La1—O10      | 2.6520 (18)         |           |
| La1—O11      | 2.631 (2)           |           |
| La1—O13      | 2.612 (2)           |           |
| La1—O14      | 2.6551 (19)         |           |
| La1—O16      | 2.674 (2)           |           |
| La1—O17      | 2.662 (2)           |           |
| O1—N1        | 1.278 (3)           |           |
| O2—N1        | 1.250 (3)           |           |
| O3—N1        | 1.210 (3)           |           |
| O4—N2        | 1.274 (3)           |           |
| O5—N2        | 1.255 (3)           |           |
| O6—N2        | 1.223 (3)           |           |
| O7—N3        | 1.269 (3)           |           |
| O8—N3        | 1.259 (3)           |           |
| O9—N3        | 1.221 (3)           |           |
| O10—N4       | 1.260 (3)           |           |
| O11—N4       | 1.275 (3)           |           |
| O12—N4       | 1.212 (3)           |           |
| O13—N5       | 1.275 (3)           |           |
| O14—N5       | 1.264 (3)           |           |
| O15—N5       | 1.216 (3)           |           |
O16—N6 1.256 (3) N13—C22 1.393 (4)
O17—N6 1.275 (3) N13—C23 1.343 (4)
O18—N6 1.218 (3) N14—C17 1.403 (4)
N7—H1 0.8600 N14—C23 1.335 (4)
N7—C6 1.387 (4) N14—C24 1.453 (5)
N7—C7 1.335 (3) N15—H9A 0.8600
N8—C1 1.395 (3) N15—H9B 0.8600
N8—C7 1.341 (4) N15—C23 1.310 (4)
N8—C8 1.455 (3) C17—C18 1.389 (4)
N9—H3A 0.8600 C17—C22 1.385 (5)
N9—H3B 0.8600 C18—H18 0.9300
N9—C7 1.313 (4) C18—C19 1.392 (4)
C1—C2 1.375 (4) C19—H19 0.9300
C1—C6 1.388 (4) C19—C20 1.386 (5)
C2—H2 0.9300 C20—H20 0.9300
C2—C3 1.388 (5) C20—C21 1.386 (4)
C3—H3 0.9300 C21—H21 0.9300
C3—C4 1.376 (6) C21—C22 1.376 (5)
C4—H4 0.9300 C24—H24A 0.9600
C4—C5 1.386 (6) C24—H24B 0.9600
C5—H5 0.9300 C24—H24C 0.9600

O1—La1—O2 47.45 (6) H3A—N9—H3B 120.0
O1—La1—O4 71.65 (6) C7—N9—H3A 120.0
O1—La1—O5 65.29 (6) C7—N9—H3B 120.0
O1—La1—O7 117.83 (6) C2—C1—N8 131.4 (3)
O1—La1—O8 109.65 (6) C2—C1—C6 122.2 (3)
O1—La1—O10 67.42 (7) C6—C1—N8 106.3 (3)
O1—La1—O14 111.39 (6) C1—C2—H2 121.8
O1—La1—O16 177.08 (6) C1—C2—C3 116.3 (4)
O1—La1—O17 132.64 (6) C3—C2—H2 121.8
O4—La1—O2 70.97 (7) C2—C3—H3 119.2
O4—La1—O5 47.94 (6) C4—C3—C2 121.5 (4)
O4—La1—O7 70.09 (6) C4—C3—H3 119.2
O4—La1—O10 134.59 (6) C3—C4—H4 118.8
O4—La1—O14 109.57 (6) C3—C4—C5 122.4 (3)
O4—La1—O16 110.05 (6) C5—C4—H4 118.8
O4—La1—O17 66.47 (6) C4—C5—H5 122.0
O5—La1—O2 99.53 (7) C6—C5—C4 116.1 (3)
O5—La1—O4 114.50 (6) C6—C5—H5 122.0
O5—La1—O10 113.90 (6) N7—C6—C1 106.8 (2)
O5—La1—O17 70.51 (6) C5—C6—N7 131.6 (3)
O7—La1—O2 74.41 (7) C5—C6—C1 121.5 (3)
O8—La1—O2 66.50 (7) N7—C7—N8 109.2 (2)
O8—La1—O4 110.80 (6) N9—C7—N8 125.0 (3)
O8—La1—O5 158.64 (6) N9—C7—N8 125.8 (3)
O8—La1—O7 47.69 (6) N8—C8—H8A 109.5
O8—La1—O10 67.32 (6) N8—C8—H8B 109.5
| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|-----------------------|--------------|-----------------------|--------------|
| O8—La1—O14            | 129.20 (7)   | N8—C8—H8C            | 109.5        |
| O8—La1—O16            | 72.16 (6)    | H8A—C8—H8B           | 109.5        |
| O8—La1—O17            | 105.15 (6)   | H8A—C8—H8C           | 109.5        |
| O10—La1—O2            | 67.23 (6)    | H8B—C8—H8C           | 109.5        |
| O10—La1—O5            | 123.81 (6)   | C14—N10—H4A          | 125.3        |
| O10—La1—O7            | 113.34 (6)   | C15—N10—H4A          | 125.3        |
| O10—La1—O14           | 103.01 (6)   | C15—N10—C14          | 109.4 (2)    |
| O10—La1—O16           | 111.76 (6)   | C9—N11—C16           | 125.3 (3)    |
| O10—La1—O17           | 158.71 (6)   | C15—N11—C9           | 108.4 (2)    |
| O11—La1—O1            | 110.99 (6)   | C15—N11—C16          | 126.2 (3)    |
| O11—La1—O2            | 111.06 (6)   | H6A—N12—H6B          | 120.0        |
| O11—La1—O4            | 177.33 (6)   | C15—N12—H6A          | 120.0        |
| O11—La1—O5            | 132.34 (6)   | C15—N12—H6B          | 120.0        |
| O11—La1—O7            | 108.55 (6)   | C10—C9—N11           | 131.5 (3)    |
| O11—La1—O8            | 69.00 (6)    | C10—C9—C14           | 122.0 (3)    |
| O11—La1—O10           | 47.98 (6)    | C14—C9—N11           | 106.6 (3)    |
| O11—La1—O14           | 69.24 (6)    | C9—C10—H10           | 121.8        |
| O11—La1—O16           | 67.30 (6)    | C9—C10—C11           | 116.4 (3)    |
| O11—La1—O17           | 110.92 (6)   | C11—C10—H10          | 121.8        |
| O13—La1—O1            | 67.53 (7)    | C10—C11—H11          | 119.2        |
| O13—La1—O2            | 110.77 (7)   | C10—C11—C12          | 121.6 (3)    |
| O13—La1—O4            | 112.56 (7)   | C12—C11—H11          | 119.2        |
| O13—La1—O5            | 66.72 (7)    | C11—C12—H12          | 119.0        |
| O13—La1—O7            | 174.63 (6)   | C13—C12—C11          | 122.1 (3)    |
| O13—La1—O8            | 132.30 (6)   | C13—C12—H12          | 119.0        |
| O13—La1—O10           | 68.46 (6)    | C12—C13—H13          | 121.9        |
| O13—La1—O11           | 68.59 (7)    | C12—C13—C14          | 116.2 (3)    |
| O13—La1—O14           | 48.26 (6)    | C14—C13—H13          | 121.9        |
| O13—La1—O16           | 109.55 (7)   | N10—C14—C9           | 106.4 (2)    |
| O13—La1—O17           | 109.53 (7)   | C13—C14—N10          | 131.9 (3)    |
| O14—La1—O2            | 158.41 (7)   | C13—C14—C9           | 121.7 (3)    |
| O14—La1—O5            | 69.15 (6)    | N10—C15—N11          | 109.2 (2)    |
| O14—La1—O7            | 126.73 (7)   | N12—C15—N10          | 125.5 (3)    |
| O14—La1—O16           | 65.90 (7)    | N12—C15—N11          | 125.2 (3)    |
| O14—La1—O17           | 65.41 (6)    | N11—C16—H16A         | 109.5        |
| O16—La1—O2            | 135.15 (7)   | N11—C16—H16B         | 109.5        |
| O16—La1—O7            | 65.09 (7)    | N11—C16—H16C         | 109.5        |
| O17—La1—O2            | 129.64 (7)   | H16A—C16—H16B        | 109.5        |
| O17—La1—O7            | 66.84 (7)    | H16A—C16—H16C        | 109.5        |
| N1—O1—La1             | 98.69 (16)   | C22—N13—H7           | 125.5        |
| N1—O2—La1             | 96.49 (15)   | C23—N13—H7           | 125.5        |
| N2—O4—La1             | 97.46 (15)   | C23—N13—C22          | 109.0 (3)    |
| N2—O5—La1             | 97.46 (15)   | C17—N14—C24          | 126.6 (3)    |
| N3—O7—La1             | 95.65 (15)   | C23—N14—C17          | 108.4 (3)    |
| N3—O8—La1             | 98.41 (14)   | C23—N14—C24          | 125.0 (3)    |
| N4—O10—La1            | 97.48 (14)   | H9A—N15—H9B          | 120.0        |
| N4—O11—La1            | 98.06 (16)   | C23—N15—H9A          | 120.0        |
### Supporting Information

| Bond | Length (Å) | Angle (°) |
|------|------------|-----------|
| N5—O13—La1 | 98.75 (15) | C23—N15—H9B | 120.0 |
| N5—O14—La1 | 96.95 (14) | C18—C17—N14 | 131.0 (3) |
| N6—O16—La1 | 97.36 (15) | C22—C17—N14 | 106.9 (3) |
| N6—O17—La1 | 97.39 (16) | C22—C17—C18 | 122.1 (3) |
| O2—N1—O1 | 116.9 (2) | C17—C18—H18 | 122.1 |
| O3—N1—O1 | 120.4 (3) | C17—C18—C19 | 115.9 (3) |
| O3—N1—O2 | 122.7 (3) | C19—C18—H18 | 122.1 |
| O5—N2—O4 | 117.1 (2) | C18—C19—H19 | 119.1 |
| O6—N2—O4 | 121.3 (2) | C20—C19—C18 | 121.8 (3) |
| O6—N2—O5 | 121.6 (2) | C20—C19—H19 | 119.1 |
| O8—N3—O7 | 117.5 (2) | C19—C20—H20 | 119.2 |
| O9—N3—O7 | 120.9 (2) | C19—C20—C21 | 121.7 (3) |
| O9—N3—O8 | 121.5 (2) | C21—C20—H20 | 119.2 |
| O10—N4—O11 | 115.9 (2) | C20—C21—H21 | 121.6 |
| O12—N4—O10 | 122.5 (2) | C22—C21—C20 | 116.8 (3) |
| O12—N4—O11 | 121.7 (3) | C22—C21—H21 | 121.6 |
| O14—N5—O13 | 116.0 (2) | C17—C22—N13 | 106.4 (3) |
| O15—N5—O13 | 121.5 (2) | C21—C22—N13 | 131.9 (3) |
| O15—N5—O14 | 122.5 (2) | C21—C22—C17 | 121.7 (3) |
| O16—N6—O17 | 117.3 (2) | N14—C23—N13 | 109.4 (3) |
| O18—N6—O16 | 122.3 (3) | N15—C23—N13 | 125.4 (3) |
| O18—N6—O17 | 120.4 (3) | N15—C23—N14 | 125.2 (3) |
| C6—N7—H1 | 125.5 | N14—C24—H24A | 109.5 |
| C7—N7—H1 | 125.5 | N14—C24—H24B | 109.5 |
| C7—N7—C6 | 109.0 (2) | N14—C24—H24C | 109.5 |
| C1—N8—C8 | 125.6 (3) | H24A—C24—H24B | 109.5 |
| C7—N8—C1 | 108.7 (2) | H24A—C24—H24C | 109.5 |
| C7—N8—C8 | 125.7 (3) | H24B—C24—H24C | 109.5 |
| La1—O1—N1—O2 | 7.3 (3) | N11—C9—C10—C11 | 178.4 (3) |
| La1—O1—N1—O3 | −171.3 (3) | N11—C9—C14—N10 | −0.7 (3) |
| La1—O2—N1—O1 | −7.1 (3) | N11—C9—C14—C13 | −179.0 (3) |
| La1—O2—N1—O3 | 171.5 (3) | C9—N11—C15—N10 | −2.1 (3) |
| La1—O4—N2—O5 | 2.2 (2) | C9—N11—C15—N12 | 179.1 (3) |
| La1—O4—N2—O6 | −175.9 (2) | C9—C10—C11—C12 | 0.7 (5) |
| La1—O5—N2—O4 | −2.2 (2) | C10—C9—C14—N10 | 178.5 (3) |
| La1—O5—N2—O6 | 175.9 (2) | C10—C9—C14—C13 | 0.2 (5) |
| La1—O7—N3—O8 | −8.4 (2) | C10—C11—C12—C13 | −0.5 (6) |
| La1—O7—N3—O9 | 171.0 (2) | C11—C12—C13—C14 | 0.1 (5) |
| La1—O8—N3—O7 | 8.7 (3) | C12—C13—C14—N10 | −177.8 (3) |
| La1—O8—N3—O9 | −170.7 (2) | C12—C13—C14—C9 | 0.0 (4) |
| La1—O10—N4—O11 | 7.7 (2) | C14—N10—C15—N11 | 1.7 (3) |
| La1—O10—N4—O12 | −172.4 (2) | C14—N10—C15—N12 | −179.5 (3) |
| La1—O11—N4—O10 | −7.8 (2) | C14—C9—C10—C11 | −0.6 (5) |
| La1—O11—N4—O12 | 172.4 (2) | C15—N10—C14—C9 | −0.6 (3) |
| La1—O13—N5—O14 | −2.3 (2) | C15—N10—C14—C13 | 177.5 (3) |
| La1—O13—N5—O15 | 177.5 (2) | C15—N11—C9—C10 | −177.4 (3) |
| La1—O14—N5—O13 | 2.3 (2) | C15—N11—C9—C14 | 1.7 (3) |
La₁—O₁₄—N₅—O₁₅  −177.6 (2)
La₁—O₁₆—N₆—O₁₇  4.3 (2)
La₁—O₁₆—N₆—O₁₈  −175.8 (2)
La₁—O₁₇—N₆—O₁₆  −4.3 (2)
La₁—O₁₇—N₆—O₁₈  175.8 (2)
N₈—C₁—C₂—C₃  −177.9 (3)
N₈—C₁—C₆—N₇  0.0 (3)
N₈—C₁—C₆—C₅  0.2 (7)
C₁—N₈—C₇—N₉  −0.3 (3)
C₁—N₈—C₇—N₉  −178.4 (3)
C₃—C₄—C₅—C₆  0.2 (7)
C₆—N₇—C₇—N₉  0.3 (3)
C₆—N₇—C₇—N₉  178.4 (3)
C₆—N₇—C₇—N₉  0.9 (5)
C₇—N₇—C₆—C₁  −0.2 (3)
C₇—N₇—C₆—C₁  −177.8 (3)
C₈—N₈—C₁—C₂  0.1 (3)
C₈—N₈—C₁—C₂  179.1 (3)
C₈—N₈—C₁—C₂  −1.9 (5)
C₈—N₈—C₁—C₂  179.1 (3)
C₈—N₈—C₁—C₂  −179.2 (3)
C₈—N₈—C₁—C₂  2.7 (5)
C₁₆—N₁₁—C₉—C₁₀  7.8 (5)
C₁₆—N₁₁—C₉—C₁₄  −173.1 (3)
C₁₆—N₁₁—Cₙ₁₅—N₁₁  172.6 (3)
C₁₆—N₁₁—Cₙ₁₅—C₁₉  −6.2 (5)
N₄—C₁₇—C₁₈—C₁₉  −178.9 (3)
N₄—C₁₇—C₁₈—C₁₉  178.2 (3)
N₄—C₁₇—C₁₉—C₁₈  1.2 (3)
N₄—C₁₇—C₁₉—C₁₈  −179.4 (3)
C₂₄—N₁₄—C₂₃—N₁₅  0.9 (5)
C₂₄—N₁₄—C₂₃—N₁₅  −179.7 (3)
C₂₄—N₁₄—C₂₃—N₁₅  0.3 (5)
C₂₄—N₁₄—C₂₃—N₁₅  −179.3 (3)
C₂₄—N₁₄—C₂₃—N₁₅  −0.3 (5)

Hydrogen-bond geometry (Å, °)

| D—H···A   | D—H  | H···A | D···A   | D—H···A |
|-----------|-------|-------|---------|---------|
| C₂₁—H₂₁···O₁₇ | 0.93  | 2.64  | 3.530 (5) | 161     |
| C₂₄⁺—H₂₄C⁺···O₁₀ | 0.96  | 2.52  | 3.348 (5) | 138     |
| N₇—H₇···O₁   | 0.86  | 2.01  | 2.819 (3) | 157     |
| N₁₀—H₄A···O₄ | 0.86  | 2.05  | 2.889 (3) | 164     |
| N₁₂—H₆A···O₆ | 0.86  | 2.10  | 2.944 (3) | 165     |
| N₁₃—H₇···O₇ | 0.86  | 2.11  | 2.920 (4) | 156     |
| N₁₅—H₉B···O₉ | 0.86  | 2.14  | 2.946 (3) | 155     |
| N₁₅⁺—H₉A⁺···O₁₇ | 0.86  | 2.32  | 3.001 (3) | 136     |

Symmetry codes: (i) x−1, −y+1/2, z−1/2; (ii) x, −y+1/2, z+1/2.