Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

# Crystal structure of bis(μ-3-nitrobenzoato)-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis[bis(3-cyanopyridine-$\kappa N^1$)(3-nitrobenzoato-$\kappa^2O,O'$)cadmium]

**Tuncer Hökelek,[a]* Nurcan Akduran,[b] Azer Özen,[c] Güventürk Uğurlu[c] and Hacali Necefoğlu[c,d]**

[a]Department of Physics, Hacettepe University, 06800 Beytepe, Ankara, Turkey, [b]SANAEM, Saray Mahallesi, Atom Caddesi, No. 27, 06980 Saray-Kazan, Ankara, Turkey, [c]Department of Chemistry, Kafkas University, 36100 Kars, Turkey, and [d]International Scientific Research Centre, Baku State University, 1148 Baku, Azerbaijan. *Correspondence e-mail: merzifon@hacettepe.edu.tr

Received 3 February 2017
Accepted 16 February 2017

Edited by M. Weil, Vienna University of Technology, Austria

**Keywords:** crystal structure; cadmium; transition metal complex; benzoic acid.

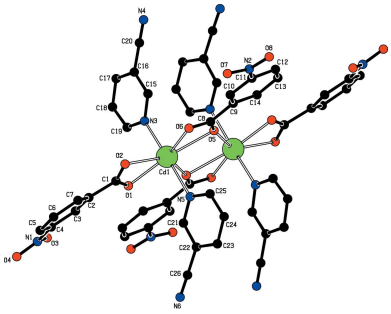
**CCDC reference**: 1533101

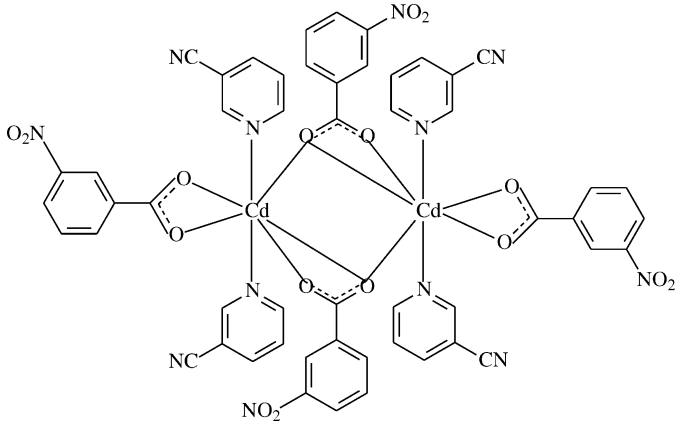
**Supporting information**: this article has supporting information at journals.iucr.org/e

The asymmetric unit of the title compound, $[Cd_2(C_7H_4NO_4)_4(C_6H_4N_2)_4]$, contains one $Cd^{II}$ atom, two 3-nitrobenzoate (NB) anions and two 3-cyanopyridine (CPy) ligands. The two CPy ligands act as monodentate N(pyridine)-bonding ligands, while the two NB anions act as bidentate ligands through the carboxylate O atoms. The centrosymmetric dinuclear complex is generated by application of inversion symmetry, whereby the $Cd^{II}$ atoms are bridged by the carboxylate O atoms of two symmetry-related NB anions, thus completing the distorted $N_2O_5$ pentagonal–bipyramidal coordination sphere of each $Cd^{II}$ atom. The benzene and pyridine rings are oriented at dihedral angles of 10.02 (7) and 5.76 (9)°, respectively. In the crystal, C—H···N hydrogen bonds link the molecules, enclosing $R_2^2(26)$ ring motifs, in which they are further linked *via* C—H···O hydrogen bonds, resulting in a three-dimensional network. In addition, π–π stacking interactions between parallel benzene rings and between parallel pyridine rings of adjacent molecules [shortest centroid-to-centroid distances = 3.885 (1) and 3.712 (1) Å, respectively], as well as a weak C—H···π interaction, may further stabilize the crystal structure.

## 1. Chemical context

In the last two decades, research on metal–organic frameworks (MOFs) has received considerable attention due to their extensive structural chemistry (Li *et al.*, 2016) and their potential applications, including gas storage, nonlinear optics and ion exchange (Carlucci *et al.*, 2003). In the syntheses of compounds having MOF structures, various carboxylate ligands have been used (Li *et al.*, 2004).






OPEN ACCESS

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.3017 (15) | Cd1—O6 | 2.3264 (15) |
| Cd1—O2 | 2.5072 (18) | Cd1—N3 | 2.3186 (17) |
| Cd1—O5 | 2.5367 (16) | Cd1—N5 | 2.3435 (17) |
| Cd1—O5$^{i}$ | 2.4716 (16) | | |

Symmetry code: (i) $-x, -y+1, -z+1$.

On the other hand, transition-metal complexes with biochemically active molecules show interesting physical and/or chemical properties, through which they may find applications in biological systems (Antolini *et al.*, 1982). Some benzoic acid derivatives, such as 4-aminobenzoic acid, have been extensively reported in coordination chemistry, as bifunctional organic ligands, due to the varieties of their coordination modes (Chen & Chen, 2002; Amiraslanov *et al.*, 1979; Hauptmann *et al.*, 2000).

The structure–function–coordination relationships of arylcarboxylate ions in $Zn^{II}$ complexes of benzoic acid derivatives change depending on the nature and position of the substituted groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the pH range and temperature of the synthesis (Shnulin *et al.*, 1981; Nadzhafov *et al.*, 1981; Antsyshkina *et al.*, 1980; Adiwidjaja *et al.*, 1978). When pyridine and its derivatives are used instead of water molecules, the structure is completely different (Catterick *et al.*, 1974).

The structures of some dinuclear complexes obtained from the reactions of transition metal(II) ions with nicotinamide (NA; $C_6H_6N_2O$) and some benzoic acid derivatives as ligands, *e.g.* $[Zn_2(C_7H_4FO_2)_4(C_6H_6N_2O)_2]\cdot C_7H_5FO_2$ [(II); Hökelek *et al.*, 2009], $[Cu_2(C_8H_7O_3)_4(C_6H_6N_2O)_2(H_2O)_2]$ [(III); Hökelek *et al.*, 2010], $[Cu_2(C_8H_5O_3)_4(C_6H_6N_2O)_4]$ [(IV); Sertçelik *et al.*, 2013], $[Mn_2(C_7H_4BrO_2)_4(C_6H_6N_2O)_2(H_2O)_2]$ [(V); Necefoğlu *et al.*, 2011] and $[Cd_2(C_7H_4ClO_2)_4(C_6H_6N_2O)_2(H_2O)_2]$ [(VI); Bozkurt *et al.*, 2013], have been determined previously. In this context, we have synthesized the $Cd^{II}$-containing title compound, bis($\mu$-3-nitrobenzoato)-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis[bis(3-cyanopyridine-$\kappa N$)(3-nitrobenzoato-$\kappa^2O,O'$)cadmium], $[Cd_2(C_7H_4NO_4)_4(C_6H_4N_2)_4]$, and report herein its crystal structure.

## 2. Structural commentary

The asymmetric unit of the title complex contains one $Cd^{II}$ atom, two 3-nitrobenzoate (NB) anions and two 3-cyanopyridine (CPy) ligands. The two CPy ligands are monodentate (through the pyridine N atoms), while both NB anions act as bidentate ligands through their carboxylate O atoms (Fig. 1). The centrosymmetric dinuclear molecule is completed by application of inversion symmerty. The $Cd^{II}$ atoms are bridged by the carboxylate O atoms of one NB anions (O6 and O5) and its symmetry-related counterpart [symmetry code: (i) $-x$, $-y+1$, $-z+1$]. Hence, this carboxylate group not only chelates to one $Cd^{II}$ atom but also bridges two $Cd^{II}$ atoms (Fig. 2). Thus, each $Cd^{II}$ atom is surrounded by three NB anions and two CPy ligands. The overall coordination sphere of the $Cd^{II}$ atom is defined by the bridging/chelating NB anions (O5, O5$^{i}$ and O6), one chelating NB anion (O1 and O2) and two 3-cyanopyridine (CPy) ligands (N3 and N5), resulting in a distorted pentagonal–bipyramidal environment. The five carboxylate O atoms (O1, O2, O5, O5$^{i}$ and O6) of the three NB anions around the $Cd^{II}$ atom form a distorted pentagonal arrangement, with an average Cd1—O bond length of 2.42 Å (Table 1). The distorted pentagonal–bipyramidal coordination is completed by pyridine atoms N3 and N5 of the CPy ligands at distances of 2.3186 (17) and 2.3435 (17) Å, respectively, in the axial positions (Table 1; Figs. 1 and 2). The Cd1 atom lies 0.1252 (1) Å above and 0.0326 (1) Å below of planar O1/O2/C1 and O5/O6/C8 carboxylate groups, respectively. The Cd1···Cd1$^{i}$ separation in the binuclear molecule is 3.9360 (15) Å and is comparable to the corresponding *M*—*M*

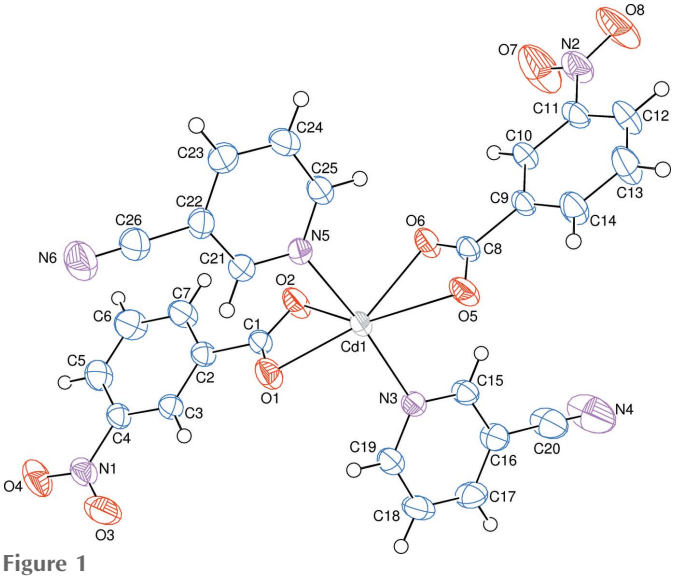



**Figure 1**
The asymmetric unit of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

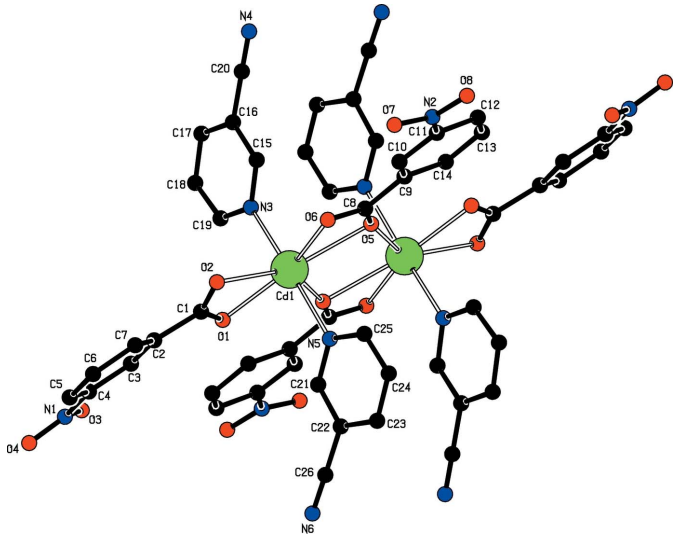



**Figure 2**
The molecular structure of the binuclear title molecule. Symmetry-related atoms are related by the symmetry code ($-x, -y+1, -z+1$). H atoms have been omitted for clarity.

**Table 2**
Hydrogen-bond geometry (Å, °).

*Cg*3 is the centroid of the N3/C15–C19 ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···O1$^{i}$ | 0.93 | 2.20 | 3.108 (3) | 167 |
| C15—H15···O2$^{ii}$ | 0.93 | 2.32 | 3.111 (3) | 143 |
| C23—H23···N4$^{iii}$ | 0.93 | 2.38 | 3.236 (5) | 154 |
| C25—H25···O6 | 0.93 | 2.58 | 3.242 (3) | 128 |
| C10—H10···*Cg*3$^{ii}$ | 0.93 | 3.26 | 4.186 (3) | 176 |

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z+1$; (iii) $x-1, y, z-1$.

distances (*M* is a metal) in the structurally related transition metal(II) complexes [7.1368 (3) Å in (III), 4.1554 (8) Å in (IV), 7.180 (2) Å in (V) and 7.1647 (3) Å in (VI)]. The metal atoms are bridged by two NA ligand N and O atoms in (III), (V) and (VI), while they are bridged by two carboxylate O atoms in (IV).

The near equalities of the C1—O1 [1.264 (3) Å], C1—O2 [1.241 (3) Å], C8—O5 [1.256 (3) Å] and C8—O6 [1.253 (3) Å] bonds in the carboxylate groups indicate delocalized bonding arrangements, rather than localized single and double bonds. The O1—Cd1—O2 and O5—Cd1—O6 bite angles are reduced to 54.33 (5) and 53.47 (5)°, respectively. The corresponding O—*M*—O (*M* is a divalent metal) angles are 60.92 (12)° in (II), 53.50 (14)° in (IV), 57.61 (8)° in (V), and 54.22 (4) and 53.32 (5)° in (VI). The dihedral angles between the planar carboxylate groups (O1/O2/C1 and O5/O6/C8) and the adjacent benzene [*A* (C2–C7) and *B* (C9–C14)] rings in the title structure are 17.18 (13) and 3.36 (12)°, respectively, while the benzene (*A* and *B*) and pyridine [*C* (N3/C15–C19) and *D* (N5/C21–C25)] rings are oriented at dihedral angles of *A*/*B* = 10.02 (7)°, *A*/*C* = 72.70 (7)°, *A*/*D* = 74.72 (7)°, *B*/*C* = 82.28 (7)°, *B*/*D* = 84.54 (8)° and *C*/*D* = 5.76 (9)°.

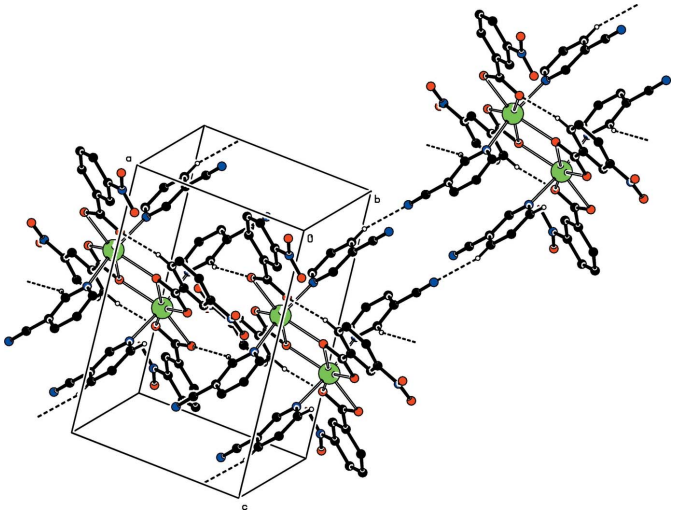



**Figure 3**
Part of the crystal structure. Intramolecular (C—$H_{cpy}$···$O_c$ and C—$H_{nb}$···$O_c$) and intermolecular (C—$H_{cpy}$···$N_{cpy}$ and C—$H_{cpy}$···$O_{nb}$) (cpy = cyanopyridine, c = carboxylate and nb = nitrobenzoate) hydrogen bonds are shown as dashed lines. Nonbonding H atoms have been omitted for clarity.

**Table 3**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[Cd_2(C_7H_4NO_4)_4(C_6H_4N_2)_4]$ |
| $M_r$ | 1305.72 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 296 |
| *a*, *b*, *c* (Å) | 8.5237 (3), 12.7145 (4), 13.0583 (5) |
| $\alpha, \beta, \gamma$ (°) | 105.022 (3), 97.347 (3), 104.866 (2) |
| *V* (Å$^3$) | 1292.12 (8) |
| *Z* | 1 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.91 |
| Crystal size (mm) | 0.28 × 0.20 × 0.18 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2012) |
| $T_{min}$, $T_{max}$ | 0.615, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 65471, 6414, 5828 |
| $R_{int}$ | 0.029 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.668 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S* | 0.029, 0.072, 1.22 |
| No. of reflections | 6414 |
| No. of parameters | 370 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.01, −0.75 |

Computer programs: *APEX2* (Bruker, 2012), *SAINT* (Bruker, 2012), *SHELXS97* (Sheldrick, 2008), *SHELXL97* (Sheldrick, 2008), *ORTEP-3* for Windows (Farrugia, 2012), *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

## 3. Supramolecular features

Intramolecular C—$H_{cpy}$···$O_c$ (cpy = cyanopyridine and c = carboxylate) and C—$H_{nb}$···$O_c$ (nb = nitrobenzoate) hydrogen bonds (Table 2) link the cyanopyridine and nitrobenzoate ligands to the carboxylate O atoms. In the crystal, C—$H_{cpy}$···$N_{cpy}$ hydrogen bonds (Table 2) link the molecules, enclosing $R_2^2(26)$ ring motifs (Bernstein *et al.*, 1995) (Fig. 3), in which they are further linked *via* additional C—$H_{cpy}$···$O_{nb}$ (nb = nitrobenzoate) hydrogen bonds (Table 2), resulting in a three-dimensional network. The $\pi$–$\pi$ contacts between parallel benzene rings and between parallel pyridine rings of adjacent molecules, *Cg*1–*Cg*2$^{i}$ and *Cg*3–*Cg*4$^{ii}$ [symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the rings *A* (atoms C2–C7), *B* (C9–C14), *C* (N3/C15–C19) and *D* (N5/C21–C25)] may further stabilize the structure, with centroid–centroid distances of 3.885 (1) and 3.712 (1) Å, respectively. A weak C—H···$\pi$ interaction (Table 2) is also observed.

## 4. Refinement

The experimental details including the crystal data, data collection and refinement are summarized in Table 3. Aromatic H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}$(H) = 1.2$U_{eq}$(C). The maximum and minimum electron densities were found at 1.43 and 0.80 Å from atoms O2 and Cd1, respectively.

## 5. Synthesis and crystallization

The title compound was prepared by the reaction of $3CdSO_4{\cdot}8H_2O$ (0.64 g, 2.5 mmol) in $H_2O$ (50 ml) and 3-cyanopyridine (0.52 g, 5 mmol) in $H_2O$ (50 ml) with sodium 3-nitrobenzoate (0.95 g, 5 mmol) in $H_2O$ (100 ml) at 333 K. The mixture was filtered and set aside to crystallize at ambient temperature for one week, giving colourless single crystals.

## Acknowledgements

The authors acknowledge the Scientific and Technological Research Application and Research Center, Sinop University, Turkey, for the use of the Bruker D8 QUEST diffractometer.

## References

Adiwidjaja, G., Rossmanith, E. & Küppers, H. (1978). *Acta Cryst.* B**34**, 3079–3083.
Amiraslanov, I. R., Mamedov, Kh. S., Movsumov, E. M., Musaev, F. N. & Nadzhafov, G. N. (1979). *Zh. Strukt. Khim.* **20**, 1075–1080.
Antolini, L., Battaglia, L. P., Corradi, A. B., Marcotrigiano, G., Menabue, L., Pellacani, G. C. & Saladini, M. (1982). *Inorg. Chem.* **21**, 1391–1395.
Antsyshkina, A. S., Chiragov, F. M. & Poray-Koshits, M. A. (1980). *Koord. Khim.* **15**, 1098–1103.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bozkurt, N., Dilek, N., Çaylak Delibaş, N., Necefoğlu, H. & Hökelek, T. (2013). *Acta Cryst.* E**69**, m389–m390.
Bruker (2012). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc. Madison, Wisconsin, USA.
Carlucci, L., Ciani, G. & Proserpio, D. M. (2003). *Coord. Chem. Rev.* **246**, 247–289.
Catterick, J., Hursthouse, M. B., New, D. B. & Thorhton, P. (1974). *J. Chem. Soc. Chem. Commun.* pp. 843–844.
Chen, H. J. & Chen, X. M. (2002). *Inorg. Chim. Acta*, **329**, 13–21.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Hauptmann, R., Kondo, M. & Kitagawa, S. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 169–172.
Hökelek, T., Süzen, Y., Tercan, B., Tenlik, E. & Necefoğlu, H. (2010). *Acta Cryst.* E**66**, m807–m808.
Hökelek, T., Yılmaz, F., Tercan, B., Özbek, F. E. & Necefoğlu, H. (2009). *Acta Cryst.* E**65**, m1608–m1609.
Li, X., Cao, R., Sun, D., Yuan, D., Bi, W., Li, X. & Wang, Y. (2004). *J. Mol. Struct.* **694**, 205–210.
Li, X., Yang, L., Zhao, L., Wang, X. L., Shao, K. Z. & Su, Z. M. (2016). *Cryst. Growth Des.* **16**, 4374–4382.
Nadzhafov, G. N., Shnulin, A. N. & Mamedov, Kh. S. (1981). *Zh. Strukt. Khim.* **22**, 124–128.
Necefoğlu, H., Özbek, F. E., Öztürk, V., Adıgüzel, V. & Hökelek, T. (2011). *Acta Cryst.* E**67**, m1128–m1129.
Sertçelik, M., Çaylak Delibaş, N., Necefoğlu, H. & Hökelek, T. (2013). *Acta Cryst.* E**69**, m290–m291.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shnulin, A. N., Nadzhafov, G. N., Amiraslanov, I. R., Usubaliev, B. T. & Mamedov, Kh. S. (1981). *Koord. Khim.* **7**, 1409–1416.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

*Acta Cryst.* (2017). E**73**, 413-416 [https://doi.org/10.1107/S2056989017002675]

# Crystal structure of bis(*μ*-3-nitrobenzoato)-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis[bis(3-cyanopyridine-$\kappa N^1$)(3-nitrobenzoato-$\kappa^2O,O'$)cadmium]

**Tuncer Hökelek, Nurcan Akduran, Azer Özen, Güventürk Uğurlu and Hacali Necefoğlu**

## Computing details

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012)′; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* for Windows (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

## Bis(*μ*-3-nitrobenzoato)-$\kappa^3O,O':O;\kappa^3O:O,O'$-bis[bis(3-cyanopyridine-$\kappa N^1$)(3-nitrobenzoato-$\kappa^2O,O'$)cadmium]

*Crystal data*

$[Cd_2(C_7H_4NO_4)_4(C_6H_4N_2)_4]$
$M_r$ = 1305.72
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 8.5237 (3) Å
$b$ = 12.7145 (4) Å
$c$ = 13.0583 (5) Å
$\alpha$ = 105.022 (3)°
$\beta$ = 97.347 (3)°
$\gamma$ = 104.866 (2)°
$V$ = 1292.12 (8) Å$^3$
$Z$ = 1
$F(000)$ = 652
$D_x$ = 1.678 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9607 reflections
$\theta$ = 3.1–28.3°
$\mu$ = 0.91 mm$^{-1}$
$T$ = 296 K
Prism, colourless
0.28 × 0.20 × 0.18 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, 2012)
$T_{min}$ = 0.615, $T_{max}$ = 0.746
65471 measured reflections
6414 independent reflections
5828 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 3.1°
$h$ = −11→11
$k$ = −16→16
$l$ = −17→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.072
$S$ = 1.22
6414 reflections
370 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.8651P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 1.01$ e Å$^{-3}$
$\Delta\rho_{min} = -0.75$ e Å$^{-3}$

*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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.151839 (18) | 0.436274 (11) | 0.419807 (11) | 0.03200 (6) |
| O1 | 0.0821 (2) | 0.25149 (13) | 0.30752 (14) | 0.0448 (4) |
| O2 | 0.3355 (2) | 0.35240 (13) | 0.30991 (15) | 0.0480 (4) |
| O3 | −0.0992 (3) | −0.15593 (16) | 0.12938 (19) | 0.0675 (6) |
| O4 | 0.0033 (3) | −0.22812 (15) | −0.00392 (17) | 0.0646 (5) |
| O5 | 0.1364 (2) | 0.61626 (13) | 0.55320 (14) | 0.0431 (4) |
| O6 | 0.3515 (2) | 0.61460 (13) | 0.47720 (13) | 0.0414 (3) |
| O7 | 0.8058 (3) | 0.9744 (2) | 0.5573 (3) | 0.1093 (12) |
| O8 | 0.7807 (3) | 1.13029 (18) | 0.6485 (3) | 0.0928 (9) |
| N1 | 0.0007 (3) | −0.14806 (16) | 0.07056 (17) | 0.0435 (4) |
| N2 | 0.7303 (3) | 1.02738 (18) | 0.6099 (2) | 0.0537 (5) |
| N3 | 0.2275 (2) | 0.37248 (14) | 0.56414 (14) | 0.0320 (3) |
| N4 | 0.6329 (5) | 0.5371 (3) | 0.8932 (3) | 0.1256 (18) |
| N5 | 0.0320 (2) | 0.48389 (15) | 0.27322 (14) | 0.0358 (4) |
| N6 | −0.3803 (3) | 0.2705 (2) | −0.0491 (2) | 0.0685 (7) |
| C1 | 0.2174 (3) | 0.26302 (16) | 0.27548 (16) | 0.0324 (4) |
| C2 | 0.2308 (3) | 0.16188 (17) | 0.19015 (17) | 0.0322 (4) |
| C3 | 0.1160 (3) | 0.05585 (17) | 0.17155 (17) | 0.0330 (4) |
| H3 | 0.0350 | 0.0469 | 0.2127 | 0.040* |
| C4 | 0.1244 (3) | −0.03626 (17) | 0.09058 (17) | 0.0347 (4) |
| C5 | 0.2408 (3) | −0.0262 (2) | 0.0267 (2) | 0.0459 (5) |
| H5 | 0.2429 | −0.0892 | −0.0279 | 0.055* |
| C6 | 0.3544 (4) | 0.0798 (2) | 0.0456 (2) | 0.0535 (6) |
| H6 | 0.4340 | 0.0886 | 0.0034 | 0.064* |
| C7 | 0.3498 (3) | 0.1736 (2) | 0.1279 (2) | 0.0447 (5) |
| H7 | 0.4274 | 0.2445 | 0.1410 | 0.054* |
| C8 | 0.2760 (2) | 0.66594 (16) | 0.53913 (16) | 0.0315 (4) |
| C9 | 0.3550 (2) | 0.79211 (16) | 0.59657 (16) | 0.0312 (4) |
| C10 | 0.5053 (3) | 0.84920 (17) | 0.57676 (18) | 0.0346 (4) |
| H10 | 0.5592 | 0.8106 | 0.5294 | 0.042* |
| C11 | 0.5721 (3) | 0.96539 (17) | 0.62989 (19) | 0.0384 (5) |
| C12 | 0.4989 (3) | 1.02590 (19) | 0.7024 (2) | 0.0491 (6) |

| | | | | |
|---|---|---|---|---|
| H12 | 0.5479 | 1.1036 | 0.7373 | 0.059* |
| C13 | 0.3506 (4) | 0.9677 (2) | 0.7217 (2) | 0.0565 (7) |
| H13 | 0.2988 | 1.0064 | 0.7706 | 0.068* |
| C14 | 0.2785 (3) | 0.8520 (2) | 0.6685 (2) | 0.0453 (5) |
| H14 | 0.1776 | 0.8140 | 0.6811 | 0.054* |
| C15 | 0.3517 (3) | 0.43881 (18) | 0.64654 (18) | 0.0360 (4) |
| H15 | 0.4061 | 0.5123 | 0.6466 | 0.043* |
| C16 | 0.4023 (3) | 0.4017 (2) | 0.73219 (19) | 0.0414 (5) |
| C17 | 0.3240 (3) | 0.2918 (2) | 0.7327 (2) | 0.0479 (6) |
| H17 | 0.3567 | 0.2653 | 0.7894 | 0.058* |
| C18 | 0.1962 (3) | 0.2229 (2) | 0.6465 (2) | 0.0503 (6) |
| H18 | 0.1411 | 0.1486 | 0.6437 | 0.060* |
| C19 | 0.1517 (3) | 0.26648 (19) | 0.56478 (19) | 0.0417 (5) |
| H19 | 0.0649 | 0.2200 | 0.5072 | 0.050* |
| C20 | 0.5330 (4) | 0.4779 (3) | 0.8215 (3) | 0.0706 (10) |
| C21 | −0.0872 (3) | 0.40583 (18) | 0.19319 (17) | 0.0375 (4) |
| H21 | −0.1240 | 0.3318 | 0.1971 | 0.045* |
| C22 | −0.1584 (3) | 0.43099 (19) | 0.10448 (17) | 0.0373 (4) |
| C23 | −0.1049 (3) | 0.5416 (2) | 0.09792 (19) | 0.0462 (5) |
| H23 | −0.1512 | 0.5609 | 0.0397 | 0.055* |
| C24 | 0.0186 (4) | 0.6213 (2) | 0.1803 (2) | 0.0541 (7) |
| H24 | 0.0579 | 0.6960 | 0.1787 | 0.065* |
| C25 | 0.0835 (3) | 0.58913 (19) | 0.26552 (19) | 0.0460 (6) |
| H25 | 0.1675 | 0.6438 | 0.3204 | 0.055* |
| C26 | −0.2833 (3) | 0.3418 (2) | 0.0192 (2) | 0.0484 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.03932 (9) | 0.02142 (7) | 0.02841 (8) | 0.00423 (6) | 0.00100 (6) | 0.00389 (5) |
| O1 | 0.0451 (9) | 0.0315 (8) | 0.0489 (9) | 0.0062 (7) | 0.0178 (7) | −0.0009 (7) |
| O2 | 0.0433 (9) | 0.0304 (8) | 0.0549 (10) | −0.0010 (7) | 0.0077 (8) | 0.0003 (7) |
| O3 | 0.0779 (14) | 0.0390 (10) | 0.0778 (14) | 0.0002 (9) | 0.0284 (12) | 0.0163 (10) |
| O4 | 0.0769 (14) | 0.0324 (9) | 0.0658 (13) | 0.0110 (9) | 0.0042 (10) | −0.0060 (8) |
| O5 | 0.0372 (8) | 0.0272 (7) | 0.0521 (9) | −0.0040 (6) | 0.0057 (7) | 0.0061 (7) |
| O6 | 0.0422 (8) | 0.0266 (7) | 0.0437 (8) | 0.0026 (6) | 0.0061 (7) | 0.0000 (6) |
| O7 | 0.0819 (17) | 0.0595 (14) | 0.155 (3) | −0.0138 (12) | 0.0739 (19) | −0.0093 (16) |
| O8 | 0.0713 (15) | 0.0345 (10) | 0.141 (2) | −0.0190 (10) | 0.0299 (15) | 0.0046 (13) |
| N1 | 0.0528 (11) | 0.0276 (9) | 0.0451 (11) | 0.0108 (8) | −0.0003 (9) | 0.0091 (8) |
| N2 | 0.0436 (11) | 0.0353 (10) | 0.0650 (14) | −0.0075 (9) | 0.0087 (10) | 0.0070 (10) |
| N3 | 0.0325 (8) | 0.0287 (8) | 0.0325 (8) | 0.0070 (7) | 0.0044 (7) | 0.0091 (7) |
| N4 | 0.136 (3) | 0.085 (2) | 0.103 (3) | −0.028 (2) | −0.077 (2) | 0.050 (2) |
| N5 | 0.0488 (10) | 0.0272 (8) | 0.0279 (8) | 0.0093 (7) | 0.0024 (7) | 0.0072 (7) |
| N6 | 0.0717 (16) | 0.0507 (14) | 0.0597 (15) | −0.0003 (12) | −0.0179 (13) | 0.0112 (12) |
| C1 | 0.0396 (10) | 0.0240 (9) | 0.0312 (9) | 0.0086 (8) | 0.0033 (8) | 0.0072 (7) |
| C2 | 0.0361 (10) | 0.0269 (9) | 0.0346 (10) | 0.0122 (8) | 0.0055 (8) | 0.0093 (8) |
| C3 | 0.0373 (10) | 0.0282 (9) | 0.0332 (10) | 0.0105 (8) | 0.0056 (8) | 0.0092 (8) |
| C4 | 0.0411 (11) | 0.0259 (9) | 0.0348 (10) | 0.0110 (8) | 0.0006 (8) | 0.0081 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0548 (14) | 0.0371 (11) | 0.0464 (13) | 0.0196 (10) | 0.0167 (11) | 0.0048 (10) |
| C6 | 0.0565 (15) | 0.0471 (14) | 0.0628 (16) | 0.0197 (12) | 0.0313 (13) | 0.0136 (12) |
| C7 | 0.0437 (12) | 0.0347 (11) | 0.0540 (14) | 0.0086 (9) | 0.0183 (10) | 0.0098 (10) |
| C8 | 0.0323 (9) | 0.0236 (9) | 0.0298 (9) | 0.0016 (7) | −0.0040 (7) | 0.0055 (7) |
| C9 | 0.0303 (9) | 0.0221 (8) | 0.0321 (9) | 0.0004 (7) | −0.0020 (7) | 0.0045 (7) |
| C10 | 0.0331 (10) | 0.0246 (9) | 0.0387 (11) | 0.0027 (7) | 0.0041 (8) | 0.0047 (8) |
| C11 | 0.0321 (10) | 0.0261 (9) | 0.0452 (12) | −0.0034 (8) | −0.0006 (9) | 0.0071 (8) |
| C12 | 0.0485 (13) | 0.0230 (10) | 0.0587 (15) | 0.0004 (9) | 0.0032 (11) | −0.0023 (10) |
| C13 | 0.0547 (15) | 0.0342 (12) | 0.0656 (17) | 0.0061 (11) | 0.0202 (13) | −0.0062 (11) |
| C14 | 0.0387 (11) | 0.0332 (11) | 0.0509 (13) | −0.0005 (9) | 0.0118 (10) | 0.0007 (10) |
| C15 | 0.0334 (10) | 0.0317 (10) | 0.0388 (11) | 0.0042 (8) | 0.0001 (8) | 0.0128 (8) |
| C16 | 0.0376 (11) | 0.0411 (12) | 0.0431 (12) | 0.0086 (9) | −0.0002 (9) | 0.0162 (10) |
| C17 | 0.0519 (14) | 0.0486 (13) | 0.0483 (13) | 0.0137 (11) | 0.0059 (11) | 0.0269 (11) |
| C18 | 0.0567 (15) | 0.0351 (12) | 0.0568 (15) | 0.0034 (10) | 0.0089 (12) | 0.0222 (11) |
| C19 | 0.0432 (12) | 0.0323 (10) | 0.0411 (12) | 0.0017 (9) | 0.0021 (9) | 0.0095 (9) |
| C20 | 0.0715 (19) | 0.0570 (17) | 0.0665 (19) | −0.0031 (14) | −0.0272 (16) | 0.0329 (15) |
| C21 | 0.0454 (12) | 0.0296 (10) | 0.0336 (10) | 0.0072 (9) | 0.0035 (9) | 0.0093 (8) |
| C22 | 0.0408 (11) | 0.0361 (11) | 0.0310 (10) | 0.0106 (9) | 0.0019 (8) | 0.0070 (8) |
| C23 | 0.0601 (15) | 0.0393 (12) | 0.0379 (11) | 0.0157 (11) | −0.0025 (10) | 0.0148 (10) |
| C24 | 0.0765 (18) | 0.0296 (11) | 0.0472 (13) | 0.0060 (11) | −0.0058 (12) | 0.0155 (10) |
| C25 | 0.0605 (15) | 0.0284 (10) | 0.0369 (11) | 0.0030 (10) | −0.0055 (10) | 0.0075 (9) |
| C26 | 0.0533 (14) | 0.0412 (12) | 0.0430 (12) | 0.0080 (11) | −0.0028 (11) | 0.0123 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O1 | 2.3017 (15) | C7—H7 | 0.9300 |
| Cd1—O2 | 2.5072 (18) | C8—C9 | 1.511 (3) |
| Cd1—O5 | 2.5367 (16) | C9—C10 | 1.393 (3) |
| Cd1—O5$^{i}$ | 2.4716 (16) | C9—C14 | 1.389 (3) |
| Cd1—O6 | 2.3264 (15) | C10—C11 | 1.387 (3) |
| Cd1—N3 | 2.3186 (17) | C10—H10 | 0.9300 |
| Cd1—N5 | 2.3435 (17) | C11—N2 | 1.470 (3) |
| Cd1—C1 | 2.733 (2) | C11—C12 | 1.377 (3) |
| O1—C1 | 1.264 (3) | C12—C13 | 1.381 (4) |
| O5—Cd1$^{i}$ | 2.4716 (16) | C12—H12 | 0.9300 |
| O5—C8 | 1.256 (3) | C13—H13 | 0.9300 |
| O6—C8 | 1.253 (3) | C14—C13 | 1.386 (3) |
| O8—N2 | 1.210 (3) | C14—H14 | 0.9300 |
| N1—O3 | 1.220 (3) | C15—C16 | 1.384 (3) |
| N1—O4 | 1.219 (3) | C15—H15 | 0.9300 |
| N1—C4 | 1.472 (3) | C16—C17 | 1.387 (3) |
| N2—O7 | 1.198 (3) | C16—C20 | 1.438 (4) |
| N3—C15 | 1.330 (3) | C17—H17 | 0.9300 |
| N3—C19 | 1.339 (3) | C18—C17 | 1.381 (4) |
| N4—C20 | 1.127 (4) | C18—H18 | 0.9300 |
| N5—C21 | 1.335 (3) | C19—C18 | 1.379 (3) |
| N5—C25 | 1.331 (3) | C19—H19 | 0.9300 |
| C1—O2 | 1.241 (3) | C21—C22 | 1.387 (3) |

| | | | |
|---|---|---|---|
| C1—C2 | 1.508 (3) | C21—H21 | 0.9300 |
| C2—C7 | 1.381 (3) | C22—C23 | 1.391 (3) |
| C3—C2 | 1.388 (3) | C22—C26 | 1.443 (3) |
| C3—C4 | 1.384 (3) | C23—C24 | 1.375 (3) |
| C3—H3 | 0.9300 | C23—H23 | 0.9300 |
| C4—C5 | 1.378 (3) | C24—H24 | 0.9300 |
| C5—C6 | 1.382 (4) | C25—C24 | 1.380 (3) |
| C5—H5 | 0.9300 | C25—H25 | 0.9300 |
| C6—H6 | 0.9300 | C26—N6 | 1.144 (3) |
| C7—C6 | 1.397 (3) | | |

| | | | |
|---|---|---|---|
| O1—Cd1—O2 | 54.33 (5) | C4—C5—H5 | 120.8 |
| O1—Cd1—O5 | 161.73 (6) | C6—C5—H5 | 120.8 |
| O1—Cd1—O5$^{i}$ | 85.39 (6) | C5—C6—C7 | 120.1 (2) |
| O1—Cd1—O6 | 144.74 (6) | C5—C6—H6 | 120.0 |
| O1—Cd1—N3 | 88.63 (6) | C7—C6—H6 | 120.0 |
| O1—Cd1—N5 | 87.92 (6) | C2—C7—C6 | 120.5 (2) |
| O1—Cd1—C1 | 27.40 (6) | C2—C7—H7 | 119.7 |
| O2—Cd1—O5 | 143.94 (5) | C6—C7—H7 | 119.7 |
| O2—Cd1—C1 | 26.95 (6) | O5—C8—C9 | 119.48 (19) |
| O5$^{i}$—Cd1—O2 | 139.57 (5) | O6—C8—O5 | 122.10 (18) |
| O5$^{i}$—Cd1—O5 | 76.40 (5) | O6—C8—C9 | 118.41 (18) |
| O5—Cd1—C1 | 170.87 (6) | C10—C9—C8 | 119.84 (19) |
| O5$^{i}$—Cd1—C1 | 112.66 (6) | C14—C9—C8 | 120.56 (19) |
| O6—Cd1—O2 | 90.60 (5) | C14—C9—C10 | 119.60 (18) |
| O6—Cd1—O5 | 53.47 (5) | C9—C10—H10 | 121.0 |
| O6—Cd1—O5$^{i}$ | 129.14 (5) | C11—C10—C9 | 117.9 (2) |
| O6—Cd1—N5 | 89.46 (6) | C11—C10—H10 | 121.0 |
| O6—Cd1—C1 | 117.41 (6) | C10—C11—N2 | 118.8 (2) |
| N3—Cd1—O2 | 93.62 (6) | C12—C11—N2 | 117.92 (19) |
| N3—Cd1—O5 | 89.29 (6) | C12—C11—C10 | 123.3 (2) |
| N3—Cd1—O5$^{i}$ | 88.16 (6) | C11—C12—C13 | 118.0 (2) |
| N3—Cd1—O6 | 98.23 (6) | C11—C12—H12 | 121.0 |
| N3—Cd1—N5 | 170.84 (6) | C13—C12—H12 | 121.0 |
| N3—Cd1—C1 | 92.02 (6) | C12—C13—C14 | 120.3 (2) |
| N5—Cd1—O2 | 91.25 (6) | C12—C13—H13 | 119.8 |
| N5—Cd1—O5 | 91.33 (6) | C14—C13—H13 | 119.8 |
| N5—Cd1—O5$^{i}$ | 83.11 (6) | C9—C14—H14 | 119.6 |
| N5—Cd1—C1 | 88.81 (6) | C13—C14—C9 | 120.9 (2) |
| C1—O1—Cd1 | 95.65 (12) | C13—C14—H14 | 119.6 |
| C1—O2—Cd1 | 86.70 (13) | N3—C15—C16 | 121.9 (2) |
| Cd1$^{i}$—O5—Cd1 | 103.60 (5) | N3—C15—H15 | 119.0 |
| C8—O5—Cd1$^{i}$ | 165.65 (15) | C16—C15—H15 | 119.0 |
| C8—O5—Cd1 | 87.27 (13) | C15—C16—C17 | 119.8 (2) |
| C8—O6—Cd1 | 97.16 (12) | C15—C16—C20 | 119.9 (2) |
| O3—N1—C4 | 118.33 (19) | C17—C16—C20 | 120.3 (2) |
| O4—N1—O3 | 123.3 (2) | C16—C17—H17 | 120.9 |
| O4—N1—C4 | 118.4 (2) | C18—C17—C16 | 118.1 (2) |

| | | | |
|---|---|---|---|
| O7—N2—O8 | 122.4 (2) | C18—C17—H17 | 120.9 |
| O7—N2—C11 | 119.0 (2) | C17—C18—H18 | 120.7 |
| O8—N2—C11 | 118.6 (2) | C19—C18—C17 | 118.7 (2) |
| C15—N3—Cd1 | 120.77 (14) | C19—C18—H18 | 120.7 |
| C15—N3—C19 | 118.26 (19) | N3—C19—C18 | 123.2 (2) |
| C19—N3—Cd1 | 120.93 (14) | N3—C19—H19 | 118.4 |
| C21—N5—Cd1 | 121.21 (14) | C18—C19—H19 | 118.4 |
| C25—N5—Cd1 | 121.09 (15) | N4—C20—C16 | 178.3 (5) |
| C25—N5—C21 | 117.68 (19) | N5—C21—C22 | 122.5 (2) |
| O1—C1—Cd1 | 56.96 (10) | N5—C21—H21 | 118.7 |
| O1—C1—C2 | 116.79 (18) | C22—C21—H21 | 118.7 |
| O2—C1—Cd1 | 66.35 (12) | C21—C22—C23 | 119.3 (2) |
| O2—C1—O1 | 123.24 (19) | C21—C22—C26 | 119.7 (2) |
| O2—C1—C2 | 120.0 (2) | C23—C22—C26 | 121.0 (2) |
| C2—C1—Cd1 | 172.89 (15) | C22—C23—H23 | 121.1 |
| C3—C2—C1 | 118.64 (19) | C24—C23—C22 | 117.9 (2) |
| C7—C2—C1 | 121.51 (19) | C24—C23—H23 | 121.1 |
| C7—C2—C3 | 119.80 (19) | C23—C24—C25 | 119.2 (2) |
| C2—C3—H3 | 120.6 | C23—C24—H24 | 120.4 |
| C4—C3—C2 | 118.7 (2) | C25—C24—H24 | 120.4 |
| C4—C3—H3 | 120.6 | N5—C25—C24 | 123.4 (2) |
| C3—C4—N1 | 118.3 (2) | N5—C25—H25 | 118.3 |
| C5—C4—N1 | 119.2 (2) | C24—C25—H25 | 118.3 |
| C5—C4—C3 | 122.4 (2) | N6—C26—C22 | 178.8 (3) |
| C4—C5—C6 | 118.5 (2) | | |

| | | | |
|---|---|---|---|
| O2—Cd1—O1—C1 | −1.60 (12) | Cd1—O1—C1—C2 | −176.08 (15) |
| O5—Cd1—O1—C1 | 179.36 (16) | Cd1—O5—C8—O6 | −0.7 (2) |
| O5$^{i}$—Cd1—O1—C1 | 174.69 (14) | Cd1$^{i}$—O5—C8—O6 | −140.5 (5) |
| O6—Cd1—O1—C1 | 5.3 (2) | Cd1—O5—C8—C9 | 178.05 (16) |
| N3—Cd1—O1—C1 | −97.04 (14) | Cd1$^{i}$—O5—C8—C9 | 38.3 (7) |
| N5—Cd1—O1—C1 | 91.44 (14) | Cd1—O6—C8—O5 | 0.8 (2) |
| O1—Cd1—O2—C1 | 1.62 (12) | Cd1—O6—C8—C9 | −177.99 (15) |
| O5—Cd1—O2—C1 | −178.89 (11) | O3—N1—C4—C3 | −3.3 (3) |
| O5$^{i}$—Cd1—O2—C1 | −4.09 (18) | O3—N1—C4—C5 | 178.5 (2) |
| O6—Cd1—O2—C1 | −174.39 (13) | O4—N1—C4—C3 | 176.7 (2) |
| N3—Cd1—O2—C1 | 87.33 (13) | O4—N1—C4—C5 | −1.5 (3) |
| N5—Cd1—O2—C1 | −84.92 (14) | Cd1—N3—C15—C16 | −178.18 (17) |
| O1—Cd1—O5—Cd1$^{i}$ | −4.8 (2) | C19—N3—C15—C16 | −0.7 (3) |
| O1—Cd1—O5—C8 | −175.30 (18) | Cd1—N3—C19—C18 | 177.4 (2) |
| O2—Cd1—O5—Cd1$^{i}$ | 176.53 (8) | C15—N3—C19—C18 | 0.0 (4) |
| O2—Cd1—O5—C8 | 6.03 (18) | Cd1—N5—C21—C22 | −178.82 (17) |
| O5$^{i}$—Cd1—O5—Cd1$^{i}$ | 0.0 | C25—N5—C21—C22 | −0.5 (3) |
| O5$^{i}$—Cd1—O5—C8 | −170.51 (16) | Cd1—N5—C25—C24 | 179.2 (2) |
| O6—Cd1—O5—Cd1$^{i}$ | 170.93 (10) | C21—N5—C25—C24 | 0.8 (4) |
| O6—Cd1—O5—C8 | 0.42 (12) | O1—C1—O2—Cd1 | −2.9 (2) |
| N3—Cd1—O5—Cd1$^{i}$ | −88.28 (7) | C2—C1—O2—Cd1 | 176.33 (17) |
| N3—Cd1—O5—C8 | 101.21 (13) | O1—C1—C2—C3 | −15.8 (3) |

| | | | |
|---|---|---|---|
| N5—Cd1—O5—Cd1$^{i}$ | 82.58 (7) | O1—C1—C2—C7 | 161.6 (2) |
| N5—Cd1—O5—C8 | −87.92 (13) | O2—C1—C2—C3 | 164.9 (2) |
| O1—Cd1—O6—C8 | 177.25 (12) | O2—C1—C2—C7 | −17.6 (3) |
| O2—Cd1—O6—C8 | −177.13 (13) | C1—C2—C7—C6 | −176.7 (2) |
| O5—Cd1—O6—C8 | −0.42 (12) | C3—C2—C7—C6 | 0.7 (4) |
| O5$^{i}$—Cd1—O6—C8 | 10.98 (16) | C4—C3—C2—C1 | 177.69 (18) |
| N3—Cd1—O6—C8 | −83.38 (13) | C4—C3—C2—C7 | 0.2 (3) |
| N5—Cd1—O6—C8 | 91.63 (13) | C2—C3—C4—N1 | −179.25 (18) |
| C1—Cd1—O6—C8 | −179.99 (12) | C2—C3—C4—C5 | −1.1 (3) |
| O1—Cd1—N3—C15 | 146.88 (17) | N1—C4—C5—C6 | 179.1 (2) |
| O1—Cd1—N3—C19 | −30.50 (17) | C3—C4—C5—C6 | 0.9 (4) |
| O2—Cd1—N3—C15 | 92.75 (17) | C4—C5—C6—C7 | 0.1 (4) |
| O2—Cd1—N3—C19 | −84.63 (17) | C2—C7—C6—C5 | −0.9 (4) |
| O5—Cd1—N3—C15 | −51.27 (16) | O5—C8—C9—C10 | −176.4 (2) |
| O5$^{i}$—Cd1—N3—C15 | −127.69 (17) | O5—C8—C9—C14 | 3.1 (3) |
| O5—Cd1—N3—C19 | 131.34 (17) | O6—C8—C9—C10 | 2.4 (3) |
| O5$^{i}$—Cd1—N3—C19 | 54.93 (17) | O6—C8—C9—C14 | −178.1 (2) |
| O6—Cd1—N3—C15 | 1.62 (17) | C8—C9—C10—C11 | 178.96 (19) |
| O6—Cd1—N3—C19 | −175.77 (17) | C14—C9—C10—C11 | −0.6 (3) |
| C1—Cd1—N3—C15 | 119.69 (17) | C8—C9—C14—C13 | 179.8 (2) |
| C1—Cd1—N3—C19 | −57.69 (17) | C10—C9—C14—C13 | −0.6 (4) |
| O1—Cd1—N5—C21 | 25.91 (17) | C9—C10—C11—N2 | −179.8 (2) |
| O1—Cd1—N5—C25 | −152.4 (2) | C9—C10—C11—C12 | 1.4 (4) |
| O2—Cd1—N5—C21 | 80.15 (18) | C10—C11—N2—O7 | −7.6 (4) |
| O2—Cd1—N5—C25 | −98.16 (19) | C10—C11—N2—O8 | 173.3 (3) |
| O5—Cd1—N5—C21 | −135.83 (17) | C12—C11—N2—O7 | 171.3 (3) |
| O5—Cd1—N5—C25 | 45.86 (19) | C12—C11—N2—O8 | −7.7 (4) |
| O5$^{i}$—Cd1—N5—C25 | 122.0 (2) | N2—C11—C12—C13 | −179.7 (3) |
| O5$^{i}$—Cd1—N5—C21 | −59.69 (17) | C10—C11—C12—C13 | −0.9 (4) |
| O6—Cd1—N5—C25 | −7.57 (19) | C11—C12—C13—C14 | −0.4 (5) |
| O6—Cd1—N5—C21 | 170.74 (18) | C9—C14—C13—C12 | 1.2 (5) |
| C1—Cd1—N5—C21 | 53.30 (18) | N3—C15—C16—C17 | 0.9 (4) |
| C1—Cd1—N5—C25 | −125.0 (2) | N3—C15—C16—C20 | −177.6 (3) |
| O1—Cd1—C1—O2 | −177.1 (2) | C15—C16—C17—C18 | −0.2 (4) |
| O2—Cd1—C1—O1 | 177.1 (2) | C20—C16—C17—C18 | 178.2 (3) |
| O5$^{i}$—Cd1—C1—O1 | −5.74 (15) | C19—C18—C17—C16 | −0.4 (4) |
| O5$^{i}$—Cd1—C1—O2 | 177.13 (13) | N3—C19—C18—C17 | 0.6 (4) |
| O6—Cd1—C1—O1 | −176.54 (13) | N5—C21—C22—C23 | −0.3 (4) |
| O6—Cd1—C1—O2 | 6.33 (15) | N5—C21—C22—C26 | 178.2 (2) |
| N3—Cd1—C1—O1 | 83.11 (14) | C21—C22—C23—C24 | 0.6 (4) |
| N3—Cd1—C1—O2 | −94.02 (14) | C26—C22—C23—C24 | −177.8 (3) |
| N5—Cd1—C1—O1 | −87.76 (14) | C22—C23—C24—C25 | −0.3 (4) |
| N5—Cd1—C1—O2 | 95.10 (14) | N5—C25—C24—C23 | −0.5 (5) |
| Cd1—O1—C1—O2 | 3.1 (2) | | |

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···O1$^{i}$ | 0.93 | 2.20 | 3.108 (3) | 167 |
| C15—H15···O2$^{ii}$ | 0.93 | 2.32 | 3.111 (3) | 143 |
| C23—H23···N4$^{iii}$ | 0.93 | 2.38 | 3.236 (5) | 154 |
| C25—H25···O6 | 0.93 | 2.58 | 3.242 (3) | 128 |
| C10—H10···*Cg*3$^{ii}$ | 0.93 | 3.26 | 4.186 (3) | 176 |

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