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# [(Nitrato-$\kappa^2O,O'$)(nitrito-$\kappa^2O,O'$)(0.25/1.75)]bis(1,10-phenanthroline-$\kappa^2N,N'$)-cadmium(II)

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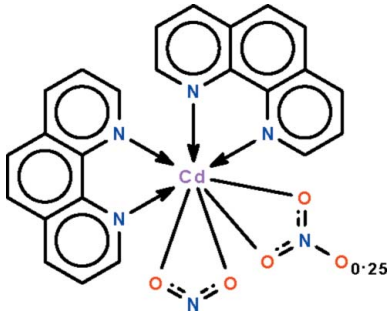
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.033; $wR$ factor = 0.073; data-to-parameter ratio = 14.9.

The reaction of cadmium nitrate and sodium nitrite in the presence of 1,10-phenanthroline yields the mixed nitrate–nitrite title complex, $[Cd(NO_2)_{1.75}(NO_3)_{0.25}(C_{12}H_8N_2)_2]$. The metal ion is bis-chelated by two *N*-heterocycles as well as by the nitrate/nitrite ions in a distorted dodecahedral $CdN_4O_4$ coordination environment. One nitrite group is ordered; the other is disordered with respect to a nitrate group (ratio 0.75:0.25) concerning the O atom that is not involved in bonding to the metal ion.

## Related literature

For the crystal structure of $[Cd(NO_3)_2(C_{12}H_8N_2)_2]$, see: Tadjarodi *et al.* (2001) and for the crystal structure of $[Cd(NO_2)_2(C_{12}H_8N_2)_2]$, see: Abedini *et al.* (2005).




## Experimental

### Crystal data

$[Cd(NO_2)_{1.75}(NO_3)_{0.25}(C_{12}H_8N_2)_2]$
$M_r$ = 568.83
Triclinic, $P\overline{1}$
$a$ = 9.1470 (4) Å
$b$ = 10.1866 (4) Å
$c$ = 13.0057 (6) Å
$\alpha$ = 76.953 (4)°
$\beta$ = 77.270 (4)°
$\gamma$ = 70.404 (4)°
$V$ = 1098.27 (8) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.04 mm$^{-1}$
$T$ = 100 K
0.30 × 0.20 × 0.10 mm

### Data collection

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
$T_{min}$ = 0.745, $T_{max}$ = 0.903
8702 measured reflections
4852 independent reflections
4256 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.073
$S$ = 1.02
4852 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.69 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Cd1—O3 | 2.355 (2) | Cd1—O1 | 2.4547 (19) |
| Cd1—N6 | 2.390 (2) | Cd1—O4 | 2.503 (2) |
| Cd1—N4 | 2.393 (2) | Cd1—O2 | 2.5041 (19) |
| Cd1—N3 | 2.418 (2) | Cd1—N5 | 2.510 (2) |

Data collection: *CrysAlis PRO* (Agilent Technologies, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2452).

## References

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# supporting information

*Acta Cryst.* (2011). E**67**, m250 [doi:10.1107/S1600536811002431]

## [(Nitrato-$\kappa^2O,O'$)(nitrito-$\kappa^2O,O'$)(0.25/1.75)]bis(1,10-phenanthroline-$\kappa^2N,N'$)cadmium(II)

**Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng**

### S1. Comment

We had previously reported the structure of the 1,10-phenanthroline adduct of cadmium nitrate. In the corresponding structure, the cadmium ion, situated on a twofold rotation axis, shows eightfold coordination, which is somewhat less common (Tadjarodi *et al.*, 2001). The compound is conveniently synthesized by the direct addition of 1,10-phenanthroline to a cadmium nitrate solution. In a similar reaction, but when nitrite ions present, a mixed nitrate/nitrite compound is obtained.

In the title compound, $Cd(NO_2)_{1.75}(NO_3)_{0.25}(C_{12}H_8N_2)_2$ (Scheme I), the metal ion also exists in an eight-coordinate distorted dodecahedral $CdN_4O_4$ geometry (Fig. 1). The metal ion is bis-chelated by two *N*-heterocycles as well as by the nitrate/nitrite ions. The molecule lies on a general position, and one nitrite group is disordered with respect to a nitrate group (ratio 0.75:0.25).

### S2. Experimental

Cadmium nitrate (1 mmol), sodium nitrite (1 mmol) and 1,10-phenanthroline (1 mmol) were loaded into a convection tube. The tube was filled with dry methanol and kept at 333 K. Colorless crystals were collected from the side arm of the tube after several days.

### S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 Å, $U_{iso}$(H) 1.2$U_{eq}$(C)] and were included in the refinement in the riding model approximation.

The structure, when refined as a dinitrite, had a high remaining peak approximately 1.2 Å away from one of the two N atoms of the nitrite groups. This site was allow to refine as an O atom of a disordered nitrate group. As the occupancy refined to nearly 1/4, its occupancy was eventually fixed as 0.25.

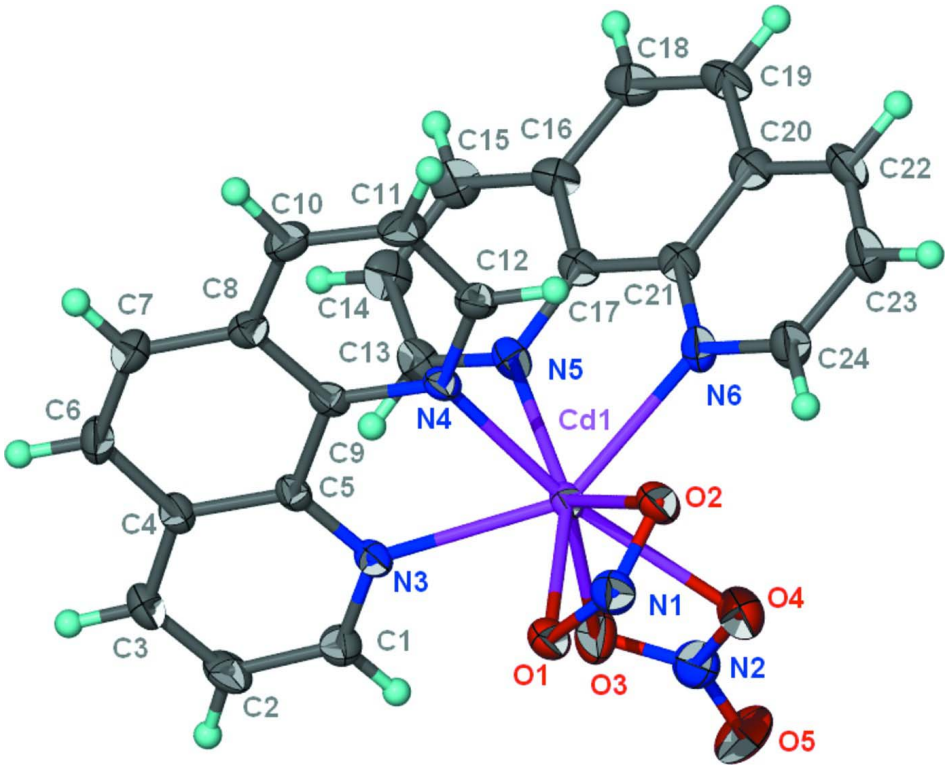


**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $Cd(NO_2)_{1.75}(NO_3)_{0.25}(C_{12}H_8N_2)_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

**[(Nitrato-$\kappa^2O,O'$)(nitrito $\kappa^2O,O'$)(0.25/1.75)]bis(1,10-phenanthroline- $\kappa^2N,N'$)cadmium(II)**

*Crystal data*

$[Cd(NO_2)_{1.75}(NO_3)_{0.25}(C_{12}H_8N_2)_2]$
$M_r$ = 568.83
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 9.1470 (4) Å
$b$ = 10.1866 (4) Å
$c$ = 13.0057 (6) Å
$\alpha$ = 76.953 (4)°
$\beta$ = 77.270 (4)°
$\gamma$ = 70.404 (4)°
$V$ = 1098.27 (8) Å$^3$
$Z$ = 2
$F(000)$ = 568
$D_x$ = 1.720 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 4883 reflections
$\theta$ = 2.4–29.3°
$\mu$ = 1.04 mm$^{-1}$
$T$ = 100 K
Irregular, colorless
0.30 × 0.20 × 0.10 mm

*Data collection*

Agilent Technologies SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent Technologies, 2010)
$T_{min}$ = 0.745, $T_{max}$ = 0.903
8702 measured reflections
4852 independent reflections
4256 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032
$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.4°
$h$ = −10→11
$k$ = −13→11
$l$ = −16→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.073$
$S = 1.02$
4852 reflections
325 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
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 0.1342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å$^{-3}$
$\Delta\rho_{min} = -0.69$ e Å$^{-3}$

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Cd1 | 0.55052 (2) | 0.243966 (18) | 0.241633 (15) | 0.01614 (7) | |
| N1 | 0.7446 (3) | −0.0427 (2) | 0.3117 (2) | 0.0230 (5) | |
| N2 | 0.8042 (3) | 0.3662 (3) | 0.1701 (2) | 0.0297 (6) | |
| N3 | 0.4863 (3) | 0.2130 (2) | 0.07978 (17) | 0.0169 (5) | |
| N4 | 0.3528 (3) | 0.1267 (2) | 0.28117 (17) | 0.0154 (5) | |
| N5 | 0.3074 (3) | 0.4518 (2) | 0.22889 (17) | 0.0178 (5) | |
| N6 | 0.4512 (3) | 0.3368 (2) | 0.40496 (18) | 0.0192 (5) | |
| O1 | 0.7414 (2) | 0.01355 (19) | 0.21528 (15) | 0.0232 (4) | |
| O2 | 0.6588 (2) | 0.0353 (2) | 0.37712 (15) | 0.0244 (5) | |
| O3 | 0.6973 (3) | 0.3783 (2) | 0.11795 (17) | 0.0324 (5) | |
| O4 | 0.7905 (3) | 0.2957 (2) | 0.26214 (17) | 0.0311 (5) | |
| O5 | 0.9091 (12) | 0.4103 (10) | 0.1371 (8) | 0.042 (2) | 0.25 |
| C1 | 0.5549 (4) | 0.2514 (3) | −0.0180 (2) | 0.0207 (6) | |
| H1 | 0.6401 | 0.2882 | −0.0259 | 0.025* | |
| C2 | 0.5079 (4) | 0.2403 (3) | −0.1101 (2) | 0.0245 (7) | |
| H2 | 0.5599 | 0.2697 | −0.1788 | 0.029* | |
| C3 | 0.3864 (4) | 0.1866 (3) | −0.1000 (2) | 0.0214 (6) | |
| H3 | 0.3534 | 0.1778 | −0.1617 | 0.026* | |
| C4 | 0.3102 (3) | 0.1446 (3) | 0.0025 (2) | 0.0172 (6) | |
| C5 | 0.3661 (3) | 0.1595 (2) | 0.0909 (2) | 0.0150 (5) | |
| C6 | 0.1825 (3) | 0.0874 (3) | 0.0203 (2) | 0.0212 (6) | |
| H6 | 0.1455 | 0.0768 | −0.0392 | 0.025* | |
| C7 | 0.1132 (4) | 0.0480 (3) | 0.1201 (2) | 0.0220 (6) | |
| H7 | 0.0260 | 0.0133 | 0.1297 | 0.026* | |
| C8 | 0.1691 (3) | 0.0577 (3) | 0.2120 (2) | 0.0181 (6) | |
| C9 | 0.2942 (3) | 0.1139 (2) | 0.1978 (2) | 0.0151 (6) | |
| C10 | 0.1059 (4) | 0.0116 (3) | 0.3171 (2) | 0.0231 (6) | |
| H10 | 0.0202 | −0.0261 | 0.3305 | 0.028* | |

| | | | | |
|---|---|---|---|---|
| C11 | 0.1695 (3) | 0.0216 (3) | 0.4007 (2) | 0.0224 (6) |
| H11 | 0.1302 | −0.0116 | 0.4722 | 0.027* |
| C12 | 0.2919 (3) | 0.0807 (3) | 0.3790 (2) | 0.0193 (6) |
| H12 | 0.3337 | 0.0884 | 0.4374 | 0.023* |
| C13 | 0.2348 (4) | 0.5050 (3) | 0.1442 (2) | 0.0208 (6) |
| H13 | 0.2824 | 0.4683 | 0.0798 | 0.025* |
| C14 | 0.0912 (4) | 0.6131 (3) | 0.1453 (2) | 0.0242 (7) |
| H14 | 0.0419 | 0.6469 | 0.0833 | 0.029* |
| C15 | 0.0235 (4) | 0.6689 (3) | 0.2363 (2) | 0.0246 (7) |
| H15 | −0.0732 | 0.7429 | 0.2381 | 0.029* |
| C16 | 0.0972 (3) | 0.6166 (3) | 0.3281 (2) | 0.0195 (6) |
| C17 | 0.2391 (3) | 0.5055 (3) | 0.3202 (2) | 0.0171 (6) |
| C18 | 0.0342 (4) | 0.6698 (3) | 0.4263 (2) | 0.0240 (7) |
| H18 | −0.0612 | 0.7451 | 0.4309 | 0.029* |
| C19 | 0.1074 (4) | 0.6156 (3) | 0.5130 (2) | 0.0240 (7) |
| H19 | 0.0644 | 0.6547 | 0.5768 | 0.029* |
| C20 | 0.2491 (4) | 0.4999 (3) | 0.5094 (2) | 0.0209 (6) |
| C21 | 0.3163 (3) | 0.4449 (3) | 0.4137 (2) | 0.0175 (6) |
| C22 | 0.3269 (4) | 0.4374 (3) | 0.5986 (2) | 0.0242 (7) |
| H22 | 0.2855 | 0.4706 | 0.6648 | 0.029* |
| C23 | 0.4628 (4) | 0.3281 (3) | 0.5883 (2) | 0.0269 (7) |
| H23 | 0.5165 | 0.2837 | 0.6477 | 0.032* |
| C24 | 0.5216 (4) | 0.2824 (3) | 0.4898 (2) | 0.0233 (6) |
| H24 | 0.6177 | 0.2080 | 0.4836 | 0.028* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.01776 (13) | 0.01855 (11) | 0.01235 (11) | −0.00468 (8) | −0.00285 (8) | −0.00377 (8) |
| N1 | 0.0219 (14) | 0.0227 (12) | 0.0237 (14) | −0.0033 (10) | −0.0042 (11) | −0.0069 (11) |
| N2 | 0.0284 (17) | 0.0363 (15) | 0.0304 (15) | −0.0163 (13) | 0.0004 (13) | −0.0124 (12) |
| N3 | 0.0190 (13) | 0.0177 (11) | 0.0145 (12) | −0.0060 (9) | −0.0005 (10) | −0.0050 (9) |
| N4 | 0.0149 (13) | 0.0173 (11) | 0.0116 (11) | −0.0024 (9) | −0.0016 (10) | −0.0021 (9) |
| N5 | 0.0247 (14) | 0.0156 (11) | 0.0137 (12) | −0.0073 (10) | −0.0027 (10) | −0.0021 (9) |
| N6 | 0.0219 (14) | 0.0186 (11) | 0.0189 (12) | −0.0043 (10) | −0.0082 (11) | −0.0043 (10) |
| O1 | 0.0218 (12) | 0.0298 (10) | 0.0171 (11) | −0.0051 (9) | −0.0027 (9) | −0.0063 (9) |
| O2 | 0.0224 (12) | 0.0309 (11) | 0.0177 (11) | −0.0022 (9) | −0.0037 (9) | −0.0081 (9) |
| O3 | 0.0370 (15) | 0.0430 (13) | 0.0277 (12) | −0.0244 (11) | −0.0071 (11) | −0.0057 (10) |
| O4 | 0.0328 (14) | 0.0357 (12) | 0.0275 (13) | −0.0096 (10) | −0.0054 (11) | −0.0110 (10) |
| O5 | 0.031 (6) | 0.053 (6) | 0.054 (6) | −0.035 (5) | 0.001 (5) | −0.009 (5) |
| C1 | 0.0216 (17) | 0.0242 (14) | 0.0180 (15) | −0.0102 (12) | −0.0011 (12) | −0.0035 (12) |
| C2 | 0.0307 (19) | 0.0293 (15) | 0.0130 (14) | −0.0130 (13) | 0.0029 (13) | −0.0027 (12) |
| C3 | 0.0274 (18) | 0.0234 (14) | 0.0154 (14) | −0.0083 (12) | −0.0044 (13) | −0.0056 (12) |
| C4 | 0.0192 (16) | 0.0164 (13) | 0.0161 (14) | −0.0030 (11) | −0.0045 (12) | −0.0048 (11) |
| C5 | 0.0160 (15) | 0.0132 (12) | 0.0140 (13) | −0.0003 (10) | −0.0034 (11) | −0.0043 (10) |
| C6 | 0.0227 (17) | 0.0243 (14) | 0.0201 (15) | −0.0068 (12) | −0.0091 (13) | −0.0056 (12) |
| C7 | 0.0182 (16) | 0.0262 (14) | 0.0248 (16) | −0.0086 (12) | −0.0045 (13) | −0.0062 (13) |
| C8 | 0.0148 (15) | 0.0194 (13) | 0.0188 (14) | −0.0032 (11) | −0.0024 (12) | −0.0038 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0148 (15) | 0.0119 (12) | 0.0143 (13) | 0.0020 (10) | −0.0024 (11) | −0.0026 (10) |
| C10 | 0.0166 (16) | 0.0298 (15) | 0.0225 (16) | −0.0090 (12) | −0.0013 (13) | −0.0021 (13) |
| C11 | 0.0176 (16) | 0.0305 (15) | 0.0147 (14) | −0.0076 (12) | 0.0008 (12) | 0.0021 (12) |
| C12 | 0.0162 (15) | 0.0235 (14) | 0.0151 (14) | −0.0032 (11) | −0.0011 (12) | −0.0027 (11) |
| C13 | 0.0279 (18) | 0.0167 (13) | 0.0167 (14) | −0.0053 (12) | −0.0049 (13) | −0.0012 (11) |
| C14 | 0.0268 (18) | 0.0201 (14) | 0.0212 (16) | −0.0029 (12) | −0.0088 (14) | 0.0038 (12) |
| C15 | 0.0252 (18) | 0.0171 (13) | 0.0278 (17) | −0.0012 (12) | −0.0071 (14) | −0.0015 (12) |
| C16 | 0.0213 (17) | 0.0152 (13) | 0.0188 (15) | −0.0046 (11) | 0.0010 (12) | −0.0020 (11) |
| C17 | 0.0195 (16) | 0.0157 (13) | 0.0165 (14) | −0.0073 (11) | 0.0004 (12) | −0.0032 (11) |
| C18 | 0.0243 (17) | 0.0176 (13) | 0.0275 (17) | −0.0053 (12) | 0.0013 (14) | −0.0053 (12) |
| C19 | 0.0297 (18) | 0.0203 (14) | 0.0213 (16) | −0.0088 (13) | 0.0046 (13) | −0.0088 (12) |
| C20 | 0.0231 (17) | 0.0207 (14) | 0.0205 (15) | −0.0101 (12) | −0.0005 (13) | −0.0038 (12) |
| C21 | 0.0214 (16) | 0.0161 (13) | 0.0155 (14) | −0.0086 (11) | −0.0007 (12) | −0.0014 (11) |
| C22 | 0.0327 (19) | 0.0289 (15) | 0.0147 (14) | −0.0134 (14) | 0.0005 (13) | −0.0087 (12) |
| C23 | 0.035 (2) | 0.0279 (15) | 0.0201 (16) | −0.0068 (14) | −0.0116 (14) | −0.0051 (13) |
| C24 | 0.0240 (17) | 0.0238 (14) | 0.0226 (16) | −0.0036 (12) | −0.0077 (13) | −0.0064 (12) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd1—O3 | 2.355 (2) | C6—H6 | 0.9500 |
| Cd1—N6 | 2.390 (2) | C7—C8 | 1.434 (4) |
| Cd1—N4 | 2.393 (2) | C7—H7 | 0.9500 |
| Cd1—N3 | 2.418 (2) | C8—C10 | 1.403 (4) |
| Cd1—O1 | 2.4547 (19) | C8—C9 | 1.403 (4) |
| Cd1—O4 | 2.503 (2) | C10—C11 | 1.377 (4) |
| Cd1—O2 | 2.5041 (19) | C10—H10 | 0.9500 |
| Cd1—N5 | 2.510 (2) | C11—C12 | 1.391 (4) |
| N1—O2 | 1.250 (3) | C11—H11 | 0.9500 |
| N1—O1 | 1.258 (3) | C12—H12 | 0.9500 |
| N2—O5 | 1.151 (9) | C13—C14 | 1.403 (4) |
| N2—O4 | 1.254 (3) | C13—H13 | 0.9500 |
| N2—O3 | 1.267 (3) | C14—C15 | 1.362 (4) |
| N3—C1 | 1.323 (3) | C14—H14 | 0.9500 |
| N3—C5 | 1.349 (3) | C15—C16 | 1.410 (4) |
| N4—C12 | 1.320 (3) | C15—H15 | 0.9500 |
| N4—C9 | 1.359 (3) | C16—C17 | 1.409 (4) |
| N5—C13 | 1.326 (3) | C16—C18 | 1.428 (4) |
| N5—C17 | 1.356 (3) | C17—C21 | 1.451 (4) |
| N6—C24 | 1.319 (3) | C18—C19 | 1.351 (4) |
| N6—C21 | 1.353 (4) | C18—H18 | 0.9500 |
| C1—C2 | 1.398 (4) | C19—C20 | 1.430 (4) |
| C1—H1 | 0.9500 | C19—H19 | 0.9500 |
| C2—C3 | 1.365 (4) | C20—C22 | 1.409 (4) |
| C2—H2 | 0.9500 | C20—C21 | 1.410 (4) |
| C3—C4 | 1.406 (4) | C22—C23 | 1.367 (4) |
| C3—H3 | 0.9500 | C22—H22 | 0.9500 |
| C4—C5 | 1.414 (3) | C23—C24 | 1.395 (4) |
| C4—C6 | 1.426 (4) | C23—H23 | 0.9500 |

| | | | |
|---|---|---|---|
| C5—C9 | 1.447 (4) | C24—H24 | 0.9500 |
| C6—C7 | 1.350 (4) | | |
| | | | |
| O3—Cd1—N6 | 111.58 (7) | N3—C5—C4 | 122.6 (2) |
| O3—Cd1—N4 | 149.81 (7) | N3—C5—C9 | 118.3 (2) |
| N6—Cd1—N4 | 90.18 (8) | C4—C5—C9 | 119.1 (2) |
| O3—Cd1—N3 | 81.88 (7) | C7—C6—C4 | 121.2 (2) |
| N6—Cd1—N3 | 145.83 (8) | C7—C6—H6 | 119.4 |
| N4—Cd1—N3 | 68.85 (7) | C4—C6—H6 | 119.4 |
| O3—Cd1—O1 | 95.42 (7) | C6—C7—C8 | 121.0 (3) |
| N6—Cd1—O1 | 127.58 (7) | C6—C7—H7 | 119.5 |
| N4—Cd1—O1 | 86.59 (7) | C8—C7—H7 | 119.5 |
| N3—Cd1—O1 | 79.44 (7) | C10—C8—C9 | 117.5 (2) |
| O3—Cd1—O4 | 51.44 (7) | C10—C8—C7 | 123.1 (3) |
| N6—Cd1—O4 | 81.44 (8) | C9—C8—C7 | 119.4 (3) |
| N4—Cd1—O4 | 157.42 (7) | N4—C9—C8 | 122.6 (2) |
| N3—Cd1—O4 | 127.41 (8) | N4—C9—C5 | 117.8 (2) |
| O1—Cd1—O4 | 82.14 (7) | C8—C9—C5 | 119.6 (2) |
| O3—Cd1—O2 | 125.56 (7) | C11—C10—C8 | 119.2 (3) |
| N6—Cd1—O2 | 77.83 (7) | C11—C10—H10 | 120.4 |
| N4—Cd1—O2 | 78.09 (7) | C8—C10—H10 | 120.4 |
| N3—Cd1—O2 | 120.90 (6) | C10—C11—C12 | 119.3 (3) |
| O1—Cd1—O2 | 50.33 (6) | C10—C11—H11 | 120.4 |
| O4—Cd1—O2 | 79.66 (7) | C12—C11—H11 | 120.4 |
| O3—Cd1—N5 | 89.71 (8) | N4—C12—C11 | 123.0 (3) |
| N6—Cd1—N5 | 67.54 (7) | N4—C12—H12 | 118.5 |
| N4—Cd1—N5 | 79.26 (7) | C11—C12—H12 | 118.5 |
| N3—Cd1—N5 | 81.80 (7) | N5—C13—C14 | 123.1 (3) |
| O1—Cd1—N5 | 159.63 (7) | N5—C13—H13 | 118.4 |
| O4—Cd1—N5 | 115.94 (7) | C14—C13—H13 | 118.4 |
| O2—Cd1—N5 | 138.17 (7) | C15—C14—C13 | 119.1 (3) |
| O2—N1—O1 | 114.4 (2) | C15—C14—H14 | 120.5 |
| O5—N2—O4 | 121.3 (5) | C13—C14—H14 | 120.5 |
| O5—N2—O3 | 124.7 (6) | C14—C15—C16 | 119.8 (3) |
| O4—N2—O3 | 113.9 (2) | C14—C15—H15 | 120.1 |
| C1—N3—C5 | 118.4 (2) | C16—C15—H15 | 120.1 |
| C1—N3—Cd1 | 124.62 (18) | C17—C16—C15 | 117.0 (3) |
| C5—N3—Cd1 | 116.90 (17) | C17—C16—C18 | 119.7 (3) |
| C12—N4—C9 | 118.3 (2) | C15—C16—C18 | 123.2 (3) |
| C12—N4—Cd1 | 123.87 (17) | N5—C17—C16 | 122.9 (2) |
| C9—N4—Cd1 | 117.69 (17) | N5—C17—C21 | 118.1 (2) |
| C13—N5—C17 | 118.0 (2) | C16—C17—C21 | 119.0 (3) |
| C13—N5—Cd1 | 125.85 (19) | C19—C18—C16 | 121.5 (3) |
| C17—N5—Cd1 | 115.91 (17) | C19—C18—H18 | 119.3 |
| C24—N6—C21 | 118.0 (3) | C16—C18—H18 | 119.3 |
| C24—N6—Cd1 | 121.76 (19) | C18—C19—C20 | 120.5 (3) |
| C21—N6—Cd1 | 120.25 (17) | C18—C19—H19 | 119.7 |
| N1—O1—Cd1 | 98.71 (15) | C20—C19—H19 | 119.7 |

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| N1—O2—Cd1 | 96.51 (15) | C22—C20—C21 | 117.6 (3) |
| N2—O3—Cd1 | 100.74 (17) | C22—C20—C19 | 122.5 (3) |
| N2—O4—Cd1 | 93.91 (16) | C21—C20—C19 | 119.9 (3) |
| N3—C1—C2 | 123.1 (3) | N6—C21—C20 | 122.6 (2) |
| N3—C1—H1 | 118.5 | N6—C21—C17 | 118.0 (2) |
| C2—C1—H1 | 118.5 | C20—C21—C17 | 119.3 (3) |
| C3—C2—C1 | 119.1 (3) | C23—C22—C20 | 119.0 (3) |
| C3—C2—H2 | 120.4 | C23—C22—H22 | 120.5 |
| C1—C2—H2 | 120.4 | C20—C22—H22 | 120.5 |
| C2—C3—C4 | 119.6 (2) | C22—C23—C24 | 119.3 (3) |
| C2—C3—H3 | 120.2 | C22—C23—H23 | 120.4 |
| C4—C3—H3 | 120.2 | C24—C23—H23 | 120.4 |
| C3—C4—C5 | 117.2 (2) | N6—C24—C23 | 123.5 (3) |
| C3—C4—C6 | 123.3 (2) | N6—C24—H24 | 118.2 |
| C5—C4—C6 | 119.5 (3) | C23—C24—H24 | 118.2 |

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| O3—Cd1—N3—C1 | 9.7 (2) | O3—N2—O4—Cd1 | 1.6 (2) |
| N6—Cd1—N3—C1 | 126.5 (2) | O3—Cd1—O4—N2 | −0.98 (16) |
| N4—Cd1—N3—C1 | −177.9 (2) | N6—Cd1—O4—N2 | −127.53 (17) |
| O1—Cd1—N3—C1 | −87.4 (2) | N4—Cd1—O4—N2 | 163.19 (18) |
| O4—Cd1—N3—C1 | −16.0 (2) | N3—Cd1—O4—N2 | 32.21 (19) |
| O2—Cd1—N3—C1 | −117.2 (2) | O1—Cd1—O4—N2 | 102.42 (17) |
| N5—Cd1—N3—C1 | 100.5 (2) | O2—Cd1—O4—N2 | 153.38 (17) |
| O3—Cd1—N3—C5 | −166.68 (19) | N5—Cd1—O4—N2 | −67.72 (18) |
| N6—Cd1—N3—C5 | −49.9 (2) | C5—N3—C1—C2 | 0.6 (4) |
| N4—Cd1—N3—C5 | 5.81 (17) | Cd1—N3—C1—C2 | −175.7 (2) |
| O1—Cd1—N3—C5 | 96.22 (18) | N3—C1—C2—C3 | −0.4 (4) |
| O4—Cd1—N3—C5 | 167.70 (16) | C1—C2—C3—C4 | 0.4 (4) |
| O2—Cd1—N3—C5 | 66.5 (2) | C2—C3—C4—C5 | −0.5 (4) |
| N5—Cd1—N3—C5 | −75.80 (18) | C2—C3—C4—C6 | −179.9 (3) |
| O3—Cd1—N4—C12 | −167.40 (19) | C1—N3—C5—C4 | −0.7 (4) |
| N6—Cd1—N4—C12 | −30.0 (2) | Cd1—N3—C5—C4 | 175.90 (19) |
| N3—Cd1—N4—C12 | 177.7 (2) | C1—N3—C5—C9 | 178.3 (2) |
| O1—Cd1—N4—C12 | 97.7 (2) | Cd1—N3—C5—C9 | −5.2 (3) |
| O4—Cd1—N4—C12 | 37.7 (3) | C3—C4—C5—N3 | 0.7 (4) |
| O2—Cd1—N4—C12 | 47.6 (2) | C6—C4—C5—N3 | −179.9 (2) |
| N5—Cd1—N4—C12 | −97.0 (2) | C3—C4—C5—C9 | −178.3 (2) |
| O3—Cd1—N4—C9 | 8.8 (3) | C6—C4—C5—C9 | 1.2 (4) |
| N6—Cd1—N4—C9 | 146.27 (18) | C3—C4—C6—C7 | 179.8 (3) |
| N3—Cd1—N4—C9 | −6.09 (17) | C5—C4—C6—C7 | 0.4 (4) |
| O1—Cd1—N4—C9 | −86.08 (18) | C4—C6—C7—C8 | −2.2 (4) |
| O4—Cd1—N4—C9 | −146.08 (19) | C6—C7—C8—C10 | −176.7 (3) |
| O2—Cd1—N4—C9 | −136.21 (19) | C6—C7—C8—C9 | 2.3 (4) |
| N5—Cd1—N4—C9 | 79.19 (18) | C12—N4—C9—C8 | 1.8 (4) |
| O3—Cd1—N5—C13 | 68.5 (2) | Cd1—N4—C9—C8 | −174.59 (18) |
| N6—Cd1—N5—C13 | −177.9 (2) | C12—N4—C9—C5 | −177.6 (2) |
| N4—Cd1—N5—C13 | −83.2 (2) | Cd1—N4—C9—C5 | 6.0 (3) |
| N3—Cd1—N5—C13 | −13.3 (2) | C10—C8—C9—N4 | −1.0 (4) |

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| O1—Cd1—N5—C13 | −36.4 (3) | C7—C8—C9—N4 | 179.8 (2) |
| O4—Cd1—N5—C13 | 114.5 (2) | C10—C8—C9—C5 | 178.4 (2) |
| O2—Cd1—N5—C13 | −141.39 (19) | C7—C8—C9—C5 | −0.7 (4) |
| O3—Cd1—N5—C17 | −117.09 (18) | N3—C5—C9—N4 | −0.5 (3) |
| N6—Cd1—N5—C17 | −3.51 (17) | C4—C5—C9—N4 | 178.5 (2) |
| N4—Cd1—N5—C17 | 91.18 (19) | N3—C5—C9—C8 | −179.9 (2) |
| N3—Cd1—N5—C17 | 161.08 (19) | C4—C5—C9—C8 | −1.0 (4) |
| O1—Cd1—N5—C17 | 138.0 (2) | C9—C8—C10—C11 | −0.8 (4) |
| O4—Cd1—N5—C17 | −71.16 (19) | C7—C8—C10—C11 | 178.3 (3) |
| O2—Cd1—N5—C17 | 33.0 (2) | C8—C10—C11—C12 | 1.8 (4) |
| O3—Cd1—N6—C24 | −99.0 (2) | C9—N4—C12—C11 | −0.8 (4) |
| N4—Cd1—N6—C24 | 102.5 (2) | Cd1—N4—C12—C11 | 175.4 (2) |
| N3—Cd1—N6—C24 | 152.85 (19) | C10—C11—C12—N4 | −1.0 (4) |
| O1—Cd1—N6—C24 | 16.6 (2) | C17—N5—C13—C14 | −0.4 (4) |
| O4—Cd1—N6—C24 | −56.5 (2) | Cd1—N5—C13—C14 | 173.9 (2) |
| O2—Cd1—N6—C24 | 24.7 (2) | N5—C13—C14—C15 | 1.4 (4) |
| N5—Cd1—N6—C24 | −179.2 (2) | C13—C14—C15—C16 | −0.7 (4) |
| O3—Cd1—N6—C21 | 83.4 (2) | C14—C15—C16—C17 | −0.9 (4) |
| N4—Cd1—N6—C21 | −75.1 (2) | C14—C15—C16—C18 | 179.7 (3) |
| N3—Cd1—N6—C21 | −24.8 (3) | C13—N5—C17—C16 | −1.4 (4) |
| O1—Cd1—N6—C21 | −160.97 (17) | Cd1—N5—C17—C16 | −176.21 (19) |
| O4—Cd1—N6—C21 | 125.9 (2) | C13—N5—C17—C21 | 178.5 (2) |
| O2—Cd1—N6—C21 | −152.9 (2) | Cd1—N5—C17—C21 | 3.7 (3) |
| N5—Cd1—N6—C21 | 3.16 (18) | C15—C16—C17—N5 | 2.0 (4) |
| O2—N1—O1—Cd1 | −1.1 (2) | C18—C16—C17—N5 | −178.5 (2) |
| O3—Cd1—O1—N1 | 133.52 (16) | C15—C16—C17—C21 | −177.9 (2) |
| N6—Cd1—O1—N1 | 10.90 (19) | C18—C16—C17—C21 | 1.6 (4) |
| N4—Cd1—O1—N1 | −76.70 (16) | C17—C16—C18—C19 | −0.3 (4) |
| N3—Cd1—O1—N1 | −145.80 (16) | C15—C16—C18—C19 | 179.2 (3) |
| O4—Cd1—O1—N1 | 83.69 (16) | C16—C18—C19—C20 | −1.6 (4) |
| O2—Cd1—O1—N1 | 0.64 (14) | C18—C19—C20—C22 | −178.1 (3) |
| N5—Cd1—O1—N1 | −122.5 (2) | C18—C19—C20—C21 | 2.2 (4) |
| O1—N1—O2—Cd1 | 1.1 (2) | C24—N6—C21—C20 | −0.4 (4) |
| O3—Cd1—O2—N1 | −64.39 (17) | Cd1—N6—C21—C20 | 177.34 (19) |
| N6—Cd1—O2—N1 | −172.34 (17) | C24—N6—C21—C17 | 179.7 (2) |
| N4—Cd1—O2—N1 | 94.86 (16) | Cd1—N6—C21—C17 | −2.6 (3) |
| N3—Cd1—O2—N1 | 38.65 (18) | C22—C20—C21—N6 | −0.5 (4) |
| O1—Cd1—O2—N1 | −0.64 (14) | C19—C20—C21—N6 | 179.1 (2) |
| O4—Cd1—O2—N1 | −88.97 (16) | C22—C20—C21—C17 | 179.4 (2) |
| N5—Cd1—O2—N1 | 153.45 (15) | C19—C20—C21—C17 | −0.9 (4) |
| O5—N2—O3—Cd1 | 175.7 (6) | N5—C17—C21—N6 | −0.9 (4) |
| O4—N2—O3—Cd1 | −1.7 (3) | C16—C17—C21—N6 | 179.0 (2) |
| N6—Cd1—O3—N2 | 59.66 (19) | N5—C17—C21—C20 | 179.1 (2) |
| N4—Cd1—O3—N2 | −167.00 (16) | C16—C17—C21—C20 | −1.0 (4) |
| N3—Cd1—O3—N2 | −152.96 (18) | C21—C20—C22—C23 | 0.4 (4) |
| O1—Cd1—O3—N2 | −74.47 (18) | C19—C20—C22—C23 | −179.3 (3) |
| O4—Cd1—O3—N2 | 0.99 (16) | C20—C22—C23—C24 | 0.6 (4) |
| O2—Cd1—O3—N2 | −30.6 (2) | C21—N6—C24—C23 | 1.5 (4) |

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| N5—Cd1—O3—N2 | 125.28 (18) | Cd1—N6—C24—C23 | −176.2 (2) |
| O5—N2—O4—Cd1 | −175.9 (6) | C22—C23—C24—N6 | −1.6 (5) |