

# Bis[1,3-bis(1-propyl-1*H*-benzimidazol-2-yl)-2-oxopropane]cadmium(II) dipicrate dimethylformamide monosolvate

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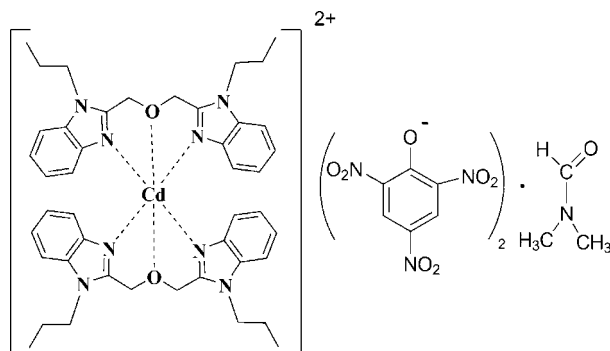
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.037;  $wR$  factor = 0.106; data-to-parameter ratio = 13.0.

In the title compound,  $[\text{Cd}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O})_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot \text{C}_3\text{H}_7\text{NO}$ , the  $\text{Cd}^{\text{II}}$  ion is coordinated by four N atoms and two O atoms from two tridentate 1,3-bis(1-propyl-1*H*-benzimidazol-2-yl)-2-oxopropane ligands in a distorted octahedral coordination environment. There are significant differences in the chemically equivalent Cd—O bond lengths [2.618 (2) Å and 2.561 (2) Å].

## Related literature

For related structures, see: Addison *et al.* (1983); Wu, Kou *et al.* (2011); Wu, Liu *et al.* (2011).



## Experimental

### Crystal data

|   |                                   |
|---|-----------------------------------|
| $[\text{Cd}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O})_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot \text{C}_3\text{H}_7\text{NO}$ | $\beta = 112.449$ (4)°            |
| $M_r = 1366.64$   | $\gamma = 97.986$ (4)°            |
| Triclinic, $P\bar{1}$   | $V = 3128$ (2) Å <sup>3</sup>     |
| $a = 14.211$ (6) Å  | $Z = 2$                           |
| $b = 14.997$ (7) Å  | Mo $K\alpha$ radiation            |
| $c = 16.190$ (7) Å  | $\mu = 0.43$ mm <sup>-1</sup>     |
| $\alpha = 94.207$ (4)°  | $T = 293$ K                       |
|   | $0.34 \times 0.29 \times 0.26$ mm |

### Data collection

|  |  |
|--|--|
| Bruker APEXII CCD diffractometer                         | 18954 measured reflections             |
| Absorption correction: multi-scan (SADABS; Bruker, 2007) | 10829 independent reflections          |
| $T_{\text{min}} = 0.867$ , $T_{\text{max}} = 0.896$      | 8918 reflections with $I > 2\sigma(I)$ |
|  | $R_{\text{int}} = 0.017$               |

### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | 3 restraints  |
| $wR(F^2) = 0.106$               | H-atom parameters constrained                       |
| $S = 0.85$                      | $\Delta\rho_{\text{max}} = 0.68$ e Å <sup>-3</sup>  |
| 10829 reflections               | $\Delta\rho_{\text{min}} = -0.51$ e Å <sup>-3</sup> |
| 835 parameters                  |   |

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5332).

## References

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**supplementary materials**

*Acta Cryst.* (2011). E67, m1461 [ doi:10.1107/S1600536811038712 ]

## Bis[1,3-bis(1-propyl-1*H*-benzimidazol-2-yl)-2-oxapropane]cadmium(II) dipicrate dimethylformamide monosolvate

H. Wu, F. Kou, F. Jia, B. Liu and J. Yuan

### Comment

Interest in bis(2-benzimidazolyl)alkanes and their derivatives is widespread (Addison *et al.*, 1983). We have previously reported the crystal structure of some related complexes (Wu, Kou *et al.*, 2011; Wu, Liu *et al.*, 2011). The asymmetric unit of the title compound, consists of a discrete [Cd(1,3-bis(1-propyl-1*H*-benzimidazol-2-yl)-2-oxapropane)<sub>2</sub>] cation, two picrate anions and a dimethylformamide solvent molecule. The cation is shown in Fig. 1. The Cd<sup>II</sup> ion is six-coordinate with a N<sub>4</sub>O<sub>2</sub> ligand set. The ligand acts as a tridentate N-donor and O-donor. The coordination geometry of the Cd<sup>II</sup> may be best described as distorted octahedral where four coordinated N atoms do not form an ideal equatorial plane. The axial sites are occupied by O1 and O2. The Cd—O bond distances indicate weak coordination. The crystal structure contains weak  $\pi\cdots\pi$  stacking interactions with centroid-to-centroid distances in the range 3.646 (3) - 3.795 (3) Å.

### Experimental

To a stirred solution of 1,3-bis(1-propyl-1*H*-benzimidazol-2-yl)-2-oxapropane (0.145 g, 0.4 mmol) in hot MeOH (5 ml), Cd(C<sub>6</sub>H<sub>2</sub>N<sub>3</sub>O<sub>7</sub>)<sub>2</sub> (0.114 g, 0.2 mmol) in MeOH (5 ml) was added. A yellow crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute Et<sub>2</sub>O, and dried *in vacuo*. The dried precipitate was dissolved in acetonitrile to give a white solution which was allowed to evaporate at room temperature. The white crystals suitable for X-ray diffraction studies were obtained after three weeks. Yield, 0.213 g (78%).

### Refinement

All H atoms were found in difference electron maps and were subsequently refined in a riding-model approximation with C—H distances ranging from 0.95 to 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2 - 1.5 U_{\text{eq}}$  of the carrier atom,

### Figures

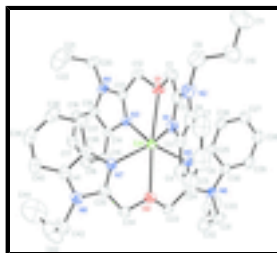


Fig. 1. The molecular structure of the cation. Hydrogen atoms have been omitted for clarity and the displacement ellipsoids are shown at the 30% probability level.

## Bis[1,3-bis(1-propyl-1H-benzimidazol-2-yl)-2-oxapropane]cadmium(II) dipicrate dimethylformamide monosolvate

### Crystal data

|   |   |
|---|---|
| $[\text{Cd}(\text{C}_{22}\text{H}_{26}\text{N}_4\text{O})_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot \text{C}_3\text{H}_7\text{NO}$ | $Z = 2$   |
| $M_r = 1366.64$   | $F(000) = 1412$   |
| Triclinic, $PT$   | $D_x = 1.451 \text{ Mg m}^{-3}$                         |
| Hall symbol: $-P 1$   | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 14.211 (6) \text{ \AA}$  | Cell parameters from 8580 reflections                   |
| $b = 14.997 (7) \text{ \AA}$  | $\theta = 2.3\text{--}25.9^\circ$                       |
| $c = 16.190 (7) \text{ \AA}$  | $\mu = 0.43 \text{ mm}^{-1}$                            |
| $\alpha = 94.207 (4)^\circ$   | $T = 293 \text{ K}$                                     |
| $\beta = 112.449 (4)^\circ$   | Block, white  |
| $\gamma = 97.986 (4)^\circ$   | $0.34 \times 0.29 \times 0.26 \text{ mm}$               |
| $V = 3128 (2) \text{ \AA}^3$  |   |

### Data collection

|   |  |
|---|--|
| Bruker APEXII CCD diffractometer                                  | 10829 independent reflections  |
| Radiation source: fine-focus sealed tube graphite                 | 8918 reflections with $I > 2\sigma(I)$                                 |
| $\omega$ scans  | $R_{\text{int}} = 0.017$   |
| Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2007) | $\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 2.1^\circ$ |
| $T_{\text{min}} = 0.867$ , $T_{\text{max}} = 0.896$               | $h = -16 \rightarrow 12$   |
| 18954 measured reflections  | $k = -17 \rightarrow 17$   |
|   | $l = -19 \rightarrow 19$   |

### Refinement

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full      | Secondary atom site location: difference Fourier map           |
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | Hydrogen site location: inferred from neighbouring sites       |
| $wR(F^2) = 0.106$               | H-atom parameters constrained                                  |
| $S = 0.85$                      | $w = 1/[\sigma^2(F_o^2) + (0.057P)^2 + 4.5262P]$               |
| 10829 reflections               | where $P = (F_o^2 + 2F_c^2)/3$                                 |
| 835 parameters                  | $(\Delta/\sigma)_{\text{max}} = 0.002$                         |
| 3 restraints                    | $\Delta\rho_{\text{max}} = 0.68 \text{ e \AA}^{-3}$            |
|                                 | $\Delta\rho_{\text{min}} = -0.51 \text{ e \AA}^{-3}$           |

*Special details*

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

**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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

|      | x             | y             | z             | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|---------------|----------------------------------|
| Cd1  | 0.710319 (17) | 0.270821 (14) | 0.087796 (14) | 0.03937 (8)                      |
| O1   | 0.6256 (2)    | 0.19157 (15)  | 0.18774 (14)  | 0.0565 (6)                       |
| O2   | 0.77052 (18)  | 0.35207 (17)  | -0.02188 (15) | 0.0564 (6)                       |
| N5   | 0.59304 (19)  | 0.34126 (16)  | -0.00581 (16) | 0.0410 (6)                       |
| N4   | 0.62449 (19)  | -0.02374 (16) | 0.07041 (17)  | 0.0432 (6)                       |
| N3   | 0.65589 (19)  | 0.11966 (16)  | 0.04931 (16)  | 0.0399 (6)                       |
| N1   | 0.7491 (2)    | 0.35220 (18)  | 0.22203 (17)  | 0.0476 (6)                       |
| N7   | 0.86953 (19)  | 0.25298 (17)  | 0.09737 (17)  | 0.0440 (6)                       |
| N6   | 0.5179 (2)    | 0.41112 (17)  | -0.12391 (18) | 0.0478 (6)                       |
| N8   | 0.9983 (2)    | 0.2479 (2)    | 0.05235 (18)  | 0.0522 (7)                       |
| C24  | 0.6019 (2)    | 0.37620 (19)  | -0.0757 (2)   | 0.0422 (7)                       |
| C13  | 0.6321 (2)    | 0.06455 (19)  | 0.10070 (19)  | 0.0386 (6)                       |
| C14  | 0.6656 (2)    | 0.0642 (2)    | -0.01885 (19) | 0.0418 (7)                       |
| C23  | 0.6946 (2)    | 0.3787 (2)    | -0.0974 (2)   | 0.0475 (7)                       |
| H23A | 0.6791        | 0.3371        | -0.1516       | 0.057*                           |
| H23B | 0.7183        | 0.4395        | -0.1067       | 0.057*                           |
| C19  | 0.6460 (2)    | -0.0258 (2)   | -0.0062 (2)   | 0.0439 (7)                       |
| C25  | 0.4979 (2)    | 0.35542 (19)  | -0.0071 (2)   | 0.0431 (7)                       |
| C35  | 0.9086 (2)    | 0.2777 (2)    | 0.0390 (2)    | 0.0441 (7)                       |
| C12  | 0.6173 (3)    | 0.0960 (2)    | 0.1835 (2)    | 0.0454 (7)                       |
| H12A | 0.5497        | 0.0681        | 0.1798        | 0.054*                           |
| H12B | 0.6699        | 0.0803        | 0.2365        | 0.054*                           |
| C40  | 1.0970 (3)    | 0.1515 (3)    | 0.1666 (3)    | 0.0693 (11)                      |
| H40  | 1.1508        | 0.1486        | 0.1478        | 0.083*                           |
| C30  | 0.4502 (2)    | 0.3986 (2)    | -0.0814 (2)   | 0.0482 (8)                       |
| C34  | 0.8581 (3)    | 0.3308 (2)    | -0.0348 (2)   | 0.0515 (8)                       |
| H34A | 0.9051        | 0.3859        | -0.0312       | 0.062*                           |
| H34B | 0.8376        | 0.2950        | -0.0932       | 0.062*                           |
| C36  | 0.9368 (2)    | 0.2022 (2)    | 0.1517 (2)    | 0.0477 (8)                       |
| C9   | 0.7450 (4)    | 0.3742 (3)    | 0.4461 (3)    | 0.0899 (15)                      |
| H9A  | 0.8111        | 0.3896        | 0.4973        | 0.108*                           |
| H9B  | 0.7159        | 0.3115        | 0.4451        | 0.108*                           |
| C18  | 0.6473 (3)    | -0.0968 (2)   | -0.0658 (2)   | 0.0553 (8)                       |

## supplementary materials

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|      |            |             |              |             |
|------|------------|-------------|--------------|-------------|
| H18  | 0.6342     | -0.1571     | -0.0572      | 0.066*      |
| C3   | 0.8162 (3) | 0.4348 (2)  | 0.2601 (2)   | 0.0538 (8)  |
| C15  | 0.6880 (3) | 0.0866 (2)  | -0.0918 (2)  | 0.0544 (8)  |
| H15  | 0.7015     | 0.1468      | -0.1005      | 0.065*      |
| C41  | 1.0176 (3) | 0.1987 (2)  | 0.1242 (2)   | 0.0519 (8)  |
| C26  | 0.4515 (3) | 0.3358 (2)  | 0.0525 (2)   | 0.0522 (8)  |
| H26  | 0.4836     | 0.3076      | 0.1025       | 0.063*      |
| N2   | 0.7619 (3) | 0.3831 (2)  | 0.36200 (19) | 0.0661 (9)  |
| C2   | 0.7189 (3) | 0.3245 (2)  | 0.2849 (2)   | 0.0523 (8)  |
| O7   | 0.1396 (3) | 0.2479 (3)  | 0.4676 (2)   | 0.1135 (13) |
| C20  | 0.6022 (3) | -0.1027 (2) | 0.1122 (3)   | 0.0619 (9)  |
| H20A | 0.5425     | -0.1439     | 0.0679       | 0.074*      |
| H20B | 0.5835     | -0.0825     | 0.1612       | 0.074*      |
| O3   | 0.2767 (3) | 0.4297 (2)  | 0.1884 (2)   | 0.0880 (9)  |
| C5   | 0.9307 (3) | 0.5714 (3)  | 0.2791 (4)   | 0.0860 (14) |
| H5   | 0.9666     | 0.6127      | 0.2566       | 0.103*      |
| C46  | 0.1506 (3) | 0.4255 (2)  | 0.2484 (2)   | 0.0566 (9)  |
| C16  | 0.6898 (3) | 0.0169 (3)  | -0.1503 (2)  | 0.0611 (9)  |
| H16  | 0.7053     | 0.0300      | -0.1995      | 0.073*      |
| C47  | 0.1043 (3) | 0.3946 (2)  | 0.3020 (2)   | 0.0595 (9)  |
| H47  | 0.0434     | 0.4125      | 0.2997       | 0.071*      |
| N9   | 0.1061 (3) | 0.4928 (3)  | 0.1904 (3)   | 0.0738 (9)  |
| C49  | 0.2395 (3) | 0.3096 (2)  | 0.3641 (3)   | 0.0660 (10) |
| H49  | 0.2701     | 0.2711      | 0.4050       | 0.079*      |
| C17  | 0.6686 (3) | -0.0735 (3) | -0.1375 (2)  | 0.0626 (10) |
| H17  | 0.6691     | -0.1194     | -0.1792      | 0.075*      |
| C8   | 0.8242 (3) | 0.4543 (3)  | 0.3482 (2)   | 0.0648 (10) |
| C6   | 0.9400 (4) | 0.5894 (4)  | 0.3674 (4)   | 0.0992 (17) |
| H6   | 0.9829     | 0.6424      | 0.4029       | 0.119*      |
| C27  | 0.3567 (3) | 0.3595 (2)  | 0.0350 (3)   | 0.0627 (10) |
| H27  | 0.3237     | 0.3473      | 0.0738       | 0.075*      |
| C37  | 0.9318 (3) | 0.1585 (2)  | 0.2232 (2)   | 0.0605 (9)  |
| H37  | 0.8778     | 0.1601      | 0.2420       | 0.073*      |
| C31  | 0.5044 (3) | 0.4585 (3)  | -0.2037 (2)  | 0.0651 (10) |
| H31A | 0.5699     | 0.4965      | -0.1936      | 0.078*      |
| H31B | 0.4547     | 0.4982      | -0.2088      | 0.078*      |
| C48  | 0.1491 (3) | 0.3357 (3)  | 0.3602 (2)   | 0.0620 (10) |
| C28  | 0.3090 (3) | 0.4019 (3)  | -0.0402 (3)  | 0.0691 (11) |
| H28  | 0.2444     | 0.4167      | -0.0506      | 0.083*      |
| C29  | 0.3542 (3) | 0.4223 (2)  | -0.0994 (3)  | 0.0629 (10) |
| H29  | 0.3219     | 0.4508      | -0.1491      | 0.075*      |
| C45  | 0.2423 (3) | 0.4005 (2)  | 0.2426 (3)   | 0.0605 (9)  |
| C10  | 0.6735 (5) | 0.4346 (4)  | 0.4583 (4)   | 0.1015 (16) |
| H10A | 0.6084     | 0.4214      | 0.4058       | 0.122*      |
| H10B | 0.7041     | 0.4976      | 0.4624       | 0.122*      |
| C7   | 0.8883 (4) | 0.5317 (3)  | 0.4038 (3)   | 0.0927 (15) |
| H7   | 0.8959     | 0.5440      | 0.4634       | 0.111*      |
| C1   | 0.6471 (3) | 0.2388 (2)  | 0.2736 (2)   | 0.0620 (10) |
| H1A  | 0.6787     | 0.2025      | 0.3205       | 0.074*      |

|      |            |             |              |             |
|------|------------|-------------|--------------|-------------|
| H1B  | 0.5838     | 0.2515      | 0.2775       | 0.074*      |
| C4   | 0.8687 (3) | 0.4930 (3)  | 0.2241 (3)   | 0.0647 (10) |
| H4   | 0.8629     | 0.4803      | 0.1651       | 0.078*      |
| O6   | 0.0156 (3) | 0.3216 (2)  | 0.4079 (2)   | 0.1010 (11) |
| N11  | 0.3791 (3) | 0.3097 (3)  | 0.3130 (4)   | 0.0902 (12) |
| C39  | 1.0916 (4) | 0.1094 (3)  | 0.2376 (3)   | 0.0791 (13) |
| H39  | 1.1436     | 0.0780      | 0.2682       | 0.095*      |
| C50  | 0.2845 (3) | 0.3403 (3)  | 0.3076 (3)   | 0.0646 (10) |
| N10  | 0.0986 (4) | 0.2994 (3)  | 0.4162 (2)   | 0.0800 (11) |
| C42  | 1.0627 (3) | 0.2656 (3)  | 0.0011 (3)   | 0.0800 (13) |
| H42A | 1.1329     | 0.2604      | 0.0391       | 0.096*      |
| H42B | 1.0639     | 0.3281      | -0.0109      | 0.096*      |
| O9   | 0.4039 (4) | 0.3093 (4)  | 0.2508 (4)   | 0.155 (2)   |
| O5   | 0.0391 (4) | 0.4708 (3)  | 0.1225 (3)   | 0.1428 (19) |
| C21  | 0.6869 (4) | -0.1531 (3) | 0.1475 (3)   | 0.0975 (16) |
| H21A | 0.6654     | -0.2035     | 0.1745       | 0.117*      |
| H21B | 0.7027     | -0.1779     | 0.0982       | 0.117*      |
| C32  | 0.4687 (5) | 0.3971 (4)  | -0.2914 (3)  | 0.1031 (17) |
| H32A | 0.4723     | 0.4336      | -0.3374      | 0.124*      |
| H32B | 0.5162     | 0.3549      | -0.2851      | 0.124*      |
| C38  | 1.0110 (3) | 0.1127 (3)  | 0.2646 (3)   | 0.0760 (12) |
| H38  | 1.0101     | 0.0827      | 0.3127       | 0.091*      |
| O8   | 0.4316 (4) | 0.2854 (4)  | 0.3832 (4)   | 0.1536 (19) |
| C22  | 0.7821 (4) | -0.0933 (4) | 0.2167 (4)   | 0.133 (2)   |
| H22A | 0.8090     | -0.0484     | 0.1882       | 0.200*      |
| H22B | 0.8333     | -0.1295     | 0.2440       | 0.200*      |
| H22C | 0.7648     | -0.0636     | 0.2622       | 0.200*      |
| O4   | 0.1450 (4) | 0.5715 (3)  | 0.2179 (3)   | 0.1296 (15) |
| C11  | 0.6530 (6) | 0.4213 (4)  | 0.5422 (4)   | 0.130 (2)   |
| H11A | 0.6107     | 0.3628      | 0.5334       | 0.195*      |
| H11B | 0.6177     | 0.4679      | 0.5536       | 0.195*      |
| H11C | 0.7175     | 0.4249      | 0.5928       | 0.195*      |
| O16  | 0.8588 (3) | 0.1721 (5)  | 0.7081 (3)   | 0.174 (2)   |
| O10  | 0.7065 (2) | 0.2162 (2)  | 0.76234 (17) | 0.0771 (8)  |
| C51  | 0.6515 (3) | 0.1857 (2)  | 0.6830 (2)   | 0.0574 (9)  |
| C55  | 0.6367 (3) | 0.1493 (3)  | 0.5255 (2)   | 0.0612 (9)  |
| H55  | 0.6687     | 0.1480      | 0.4851       | 0.073*      |
| O15  | 0.8389 (3) | 0.2477 (3)  | 0.6001 (3)   | 0.1191 (13) |
| O11  | 0.5237 (2) | 0.1976 (2)  | 0.7776 (2)   | 0.0816 (8)  |
| C52  | 0.5414 (3) | 0.1541 (2)  | 0.6456 (2)   | 0.0591 (9)  |
| C56  | 0.6933 (3) | 0.1775 (3)  | 0.6148 (2)   | 0.0584 (9)  |
| N12  | 0.4861 (3) | 0.1511 (3)  | 0.7042 (2)   | 0.0766 (10) |
| N13  | 0.4700 (3) | 0.0922 (3)  | 0.4015 (2)   | 0.0812 (11) |
| C54  | 0.5313 (3) | 0.1226 (2)  | 0.4958 (2)   | 0.0618 (10) |
| C53  | 0.4841 (3) | 0.1235 (3)  | 0.5559 (3)   | 0.0653 (10) |
| H53  | 0.4131     | 0.1034      | 0.5356       | 0.078*      |
| O14  | 0.5141 (3) | 0.0912 (3)  | 0.3502 (2)   | 0.1057 (12) |
| N14  | 0.8046 (3) | 0.2030 (3)  | 0.6435 (3)   | 0.0885 (12) |
| O12  | 0.4024 (3) | 0.1012 (3)  | 0.6781 (3)   | 0.1429 (19) |

## supplementary materials

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|      |            |             |             |             |
|------|------------|-------------|-------------|-------------|
| O13  | 0.3766 (3) | 0.0677 (3)  | 0.3776 (2)  | 0.1141 (13) |
| C59  | 0.8829 (4) | 0.1286 (4)  | 0.4491 (3)  | 0.0858 (13) |
| H59  | 0.9329     | 0.1795      | 0.4578      | 0.103*      |
| O17  | 0.8046 (3) | 0.1163 (3)  | 0.3811 (2)  | 0.1279 (15) |
| N15  | 0.9016 (3) | 0.0747 (3)  | 0.5112 (2)  | 0.0774 (10) |
| C58  | 0.9977 (4) | 0.0980 (4)  | 0.5908 (3)  | 0.1079 (18) |
| H58A | 1.0419     | 0.1477      | 0.5822      | 0.162*      |
| H58B | 1.0316     | 0.0463      | 0.6004      | 0.162*      |
| H58C | 0.9831     | 0.1153      | 0.6423      | 0.162*      |
| C57  | 0.8279 (4) | -0.0031 (4) | 0.5063 (4)  | 0.1088 (17) |
| H57A | 0.7687     | -0.0103     | 0.4501      | 0.163*      |
| H57B | 0.8065     | 0.0050      | 0.5554      | 0.163*      |
| H57C | 0.8590     | -0.0564     | 0.5099      | 0.163*      |
| C33  | 0.3641 (5) | 0.3450 (5)  | -0.3223 (4) | 0.146 (3)   |
| H33A | 0.3613     | 0.3037      | -0.2804     | 0.219*      |
| H33B | 0.3456     | 0.3113      | -0.3807     | 0.219*      |
| H33C | 0.3166     | 0.3857      | -0.3261     | 0.219*      |
| C44  | 1.0208 (8) | 0.1080 (5)  | -0.0776 (6) | 0.202 (4)   |
| H44A | 1.0793     | 0.0964      | -0.0277     | 0.303*      |
| H44B | 1.0170     | 0.0755      | -0.1325     | 0.303*      |
| H44C | 0.9586     | 0.0880      | -0.0687     | 0.303*      |
| C43  | 1.0326 (6) | 0.2079 (5)  | -0.0837 (4) | 0.151 (3)   |
| H43A | 0.9673     | 0.2203      | -0.1256     | 0.181*      |
| H43B | 1.0840     | 0.2240      | -0.1084     | 0.181*      |

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

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$    | $U^{13}$     | $U^{23}$    |
|-----|--------------|--------------|--------------|-------------|--------------|-------------|
| Cd1 | 0.04318 (14) | 0.03691 (13) | 0.03939 (13) | 0.00771 (9) | 0.01700 (10) | 0.00926 (9) |
| O1  | 0.0901 (18)  | 0.0450 (13)  | 0.0430 (12)  | 0.0161 (12) | 0.0340 (12)  | 0.0089 (10) |
| O2  | 0.0504 (13)  | 0.0819 (17)  | 0.0476 (13)  | 0.0251 (12) | 0.0233 (11)  | 0.0269 (12) |
| N5  | 0.0439 (14)  | 0.0331 (13)  | 0.0463 (14)  | 0.0078 (11) | 0.0171 (12)  | 0.0102 (11) |
| N4  | 0.0458 (15)  | 0.0341 (13)  | 0.0470 (14)  | 0.0050 (11) | 0.0155 (12)  | 0.0103 (11) |
| N3  | 0.0456 (14)  | 0.0345 (13)  | 0.0401 (13)  | 0.0062 (11) | 0.0171 (11)  | 0.0089 (10) |
| N1  | 0.0519 (16)  | 0.0475 (15)  | 0.0414 (14)  | 0.0143 (13) | 0.0149 (12)  | 0.0048 (12) |
| N7  | 0.0402 (14)  | 0.0464 (15)  | 0.0449 (14)  | 0.0081 (12) | 0.0155 (12)  | 0.0095 (11) |
| N6  | 0.0484 (16)  | 0.0422 (15)  | 0.0503 (15)  | 0.0104 (12) | 0.0144 (13)  | 0.0167 (12) |
| N8  | 0.0436 (15)  | 0.0629 (18)  | 0.0515 (16)  | 0.0108 (13) | 0.0207 (13)  | 0.0043 (13) |
| C24 | 0.0446 (17)  | 0.0333 (15)  | 0.0436 (16)  | 0.0077 (13) | 0.0110 (14)  | 0.0084 (13) |
| C13 | 0.0324 (15)  | 0.0386 (16)  | 0.0393 (15)  | 0.0052 (12) | 0.0080 (12)  | 0.0092 (12) |
| C14 | 0.0414 (17)  | 0.0402 (17)  | 0.0380 (15)  | 0.0038 (13) | 0.0112 (13)  | 0.0020 (12) |
| C23 | 0.0500 (19)  | 0.0512 (19)  | 0.0437 (17)  | 0.0140 (15) | 0.0172 (15)  | 0.0191 (14) |
| C19 | 0.0424 (17)  | 0.0415 (17)  | 0.0425 (16)  | 0.0069 (14) | 0.0112 (14)  | 0.0055 (13) |
| C25 | 0.0411 (17)  | 0.0287 (15)  | 0.0540 (18)  | 0.0032 (13) | 0.0149 (14)  | 0.0011 (13) |
| C35 | 0.0383 (17)  | 0.0479 (18)  | 0.0427 (16)  | 0.0027 (14) | 0.0147 (14)  | 0.0022 (14) |
| C12 | 0.0488 (18)  | 0.0422 (17)  | 0.0445 (17)  | 0.0049 (14) | 0.0183 (14)  | 0.0102 (13) |
| C40 | 0.057 (2)    | 0.074 (3)    | 0.070 (2)    | 0.026 (2)   | 0.0135 (19)  | 0.000 (2)   |
| C30 | 0.0444 (18)  | 0.0368 (17)  | 0.0585 (19)  | 0.0071 (14) | 0.0149 (15)  | 0.0082 (14) |



|     |             |             |             |              |             |              |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| C34 | 0.0473 (19) | 0.065 (2)   | 0.0464 (18) | 0.0106 (16)  | 0.0214 (15) | 0.0152 (15)  |
| C36 | 0.0429 (18) | 0.0424 (17) | 0.0464 (17) | 0.0027 (14)  | 0.0080 (14) | 0.0005 (14)  |
| C9  | 0.140 (4)   | 0.077 (3)   | 0.049 (2)   | 0.028 (3)    | 0.032 (3)   | 0.003 (2)    |
| C18 | 0.058 (2)   | 0.0406 (18) | 0.062 (2)   | 0.0090 (16)  | 0.0184 (17) | 0.0016 (15)  |
| C3  | 0.0439 (19) | 0.049 (2)   | 0.060 (2)   | 0.0174 (16)  | 0.0089 (16) | 0.0037 (16)  |
| C15 | 0.067 (2)   | 0.052 (2)   | 0.0445 (18) | 0.0086 (17)  | 0.0221 (17) | 0.0090 (15)  |
| C41 | 0.0464 (19) | 0.052 (2)   | 0.0484 (18) | 0.0109 (15)  | 0.0095 (15) | -0.0014 (15) |
| C26 | 0.056 (2)   | 0.0398 (18) | 0.062 (2)   | 0.0074 (15)  | 0.0249 (17) | 0.0068 (15)  |
| N2  | 0.090 (2)   | 0.061 (2)   | 0.0423 (16) | 0.0214 (18)  | 0.0193 (16) | -0.0002 (14) |
| C2  | 0.067 (2)   | 0.051 (2)   | 0.0390 (17) | 0.0260 (17)  | 0.0160 (16) | 0.0048 (14)  |
| O7  | 0.154 (4)   | 0.109 (3)   | 0.073 (2)   | -0.001 (2)   | 0.045 (2)   | 0.035 (2)    |
| C20 | 0.075 (3)   | 0.0435 (19) | 0.067 (2)   | 0.0055 (18)  | 0.029 (2)   | 0.0182 (17)  |
| O3  | 0.106 (2)   | 0.081 (2)   | 0.115 (2)   | 0.0236 (18)  | 0.079 (2)   | 0.0353 (18)  |
| C5  | 0.057 (3)   | 0.065 (3)   | 0.127 (4)   | 0.003 (2)    | 0.032 (3)   | 0.003 (3)    |
| C46 | 0.055 (2)   | 0.052 (2)   | 0.062 (2)   | 0.0019 (16)  | 0.0240 (18) | 0.0107 (16)  |
| C16 | 0.069 (2)   | 0.071 (3)   | 0.0467 (19) | 0.0126 (19)  | 0.0264 (18) | 0.0042 (17)  |
| C47 | 0.059 (2)   | 0.055 (2)   | 0.066 (2)   | -0.0011 (17) | 0.0298 (19) | 0.0045 (18)  |
| N9  | 0.074 (2)   | 0.071 (2)   | 0.080 (2)   | -0.0010 (19) | 0.036 (2)   | 0.0223 (19)  |
| C49 | 0.082 (3)   | 0.047 (2)   | 0.057 (2)   | 0.0055 (19)  | 0.017 (2)   | 0.0100 (17)  |
| C17 | 0.065 (2)   | 0.067 (2)   | 0.052 (2)   | 0.0187 (19)  | 0.0196 (18) | -0.0076 (18) |
| C8  | 0.067 (2)   | 0.057 (2)   | 0.055 (2)   | 0.0186 (19)  | 0.0077 (18) | -0.0056 (17) |
| C6  | 0.077 (3)   | 0.074 (3)   | 0.114 (4)   | 0.000 (3)    | 0.014 (3)   | -0.024 (3)   |
| C27 | 0.061 (2)   | 0.053 (2)   | 0.083 (3)   | 0.0084 (18)  | 0.039 (2)   | 0.0047 (19)  |
| C37 | 0.061 (2)   | 0.058 (2)   | 0.055 (2)   | 0.0074 (18)  | 0.0139 (17) | 0.0173 (17)  |
| C31 | 0.066 (2)   | 0.065 (2)   | 0.062 (2)   | 0.0199 (19)  | 0.0173 (19) | 0.0303 (19)  |
| C48 | 0.078 (3)   | 0.053 (2)   | 0.053 (2)   | -0.0021 (19) | 0.0301 (19) | 0.0024 (17)  |
| C28 | 0.052 (2)   | 0.062 (2)   | 0.099 (3)   | 0.0213 (19)  | 0.032 (2)   | 0.013 (2)    |
| C29 | 0.052 (2)   | 0.056 (2)   | 0.080 (3)   | 0.0195 (18)  | 0.0204 (19) | 0.0203 (19)  |
| C45 | 0.067 (2)   | 0.049 (2)   | 0.068 (2)   | 0.0018 (18)  | 0.033 (2)   | 0.0064 (17)  |
| C10 | 0.136 (5)   | 0.095 (4)   | 0.091 (3)   | 0.024 (3)    | 0.065 (3)   | 0.002 (3)    |
| C7  | 0.089 (3)   | 0.078 (3)   | 0.081 (3)   | 0.011 (3)    | 0.008 (3)   | -0.023 (3)   |
| C1  | 0.093 (3)   | 0.056 (2)   | 0.050 (2)   | 0.021 (2)    | 0.039 (2)   | 0.0073 (16)  |
| C4  | 0.049 (2)   | 0.058 (2)   | 0.084 (3)   | 0.0136 (18)  | 0.022 (2)   | 0.005 (2)    |
| O6  | 0.131 (3)   | 0.093 (2)   | 0.108 (3)   | 0.002 (2)    | 0.086 (3)   | 0.0066 (19)  |
| N11 | 0.089 (3)   | 0.069 (2)   | 0.118 (4)   | 0.026 (2)    | 0.042 (3)   | 0.024 (2)    |
| C39 | 0.071 (3)   | 0.070 (3)   | 0.078 (3)   | 0.030 (2)    | 0.003 (2)   | 0.014 (2)    |
| C50 | 0.064 (2)   | 0.049 (2)   | 0.081 (3)   | 0.0105 (18)  | 0.029 (2)   | 0.0046 (19)  |
| N10 | 0.112 (3)   | 0.065 (2)   | 0.064 (2)   | -0.007 (2)   | 0.044 (2)   | 0.0070 (18)  |
| C42 | 0.063 (3)   | 0.114 (4)   | 0.080 (3)   | 0.026 (2)    | 0.044 (2)   | 0.014 (3)    |
| O9  | 0.151 (4)   | 0.203 (5)   | 0.188 (5)   | 0.109 (4)    | 0.114 (4)   | 0.081 (4)    |
| O5  | 0.151 (4)   | 0.106 (3)   | 0.096 (3)   | -0.003 (3)   | -0.025 (3)  | 0.026 (2)    |
| C21 | 0.113 (4)   | 0.083 (3)   | 0.089 (3)   | 0.027 (3)    | 0.024 (3)   | 0.036 (3)    |
| C32 | 0.129 (5)   | 0.094 (4)   | 0.066 (3)   | 0.032 (3)    | 0.011 (3)   | 0.028 (3)    |
| C38 | 0.075 (3)   | 0.069 (3)   | 0.067 (2)   | 0.015 (2)    | 0.006 (2)   | 0.023 (2)    |
| O8  | 0.122 (4)   | 0.160 (4)   | 0.189 (5)   | 0.077 (3)    | 0.047 (3)   | 0.075 (4)    |
| C22 | 0.119 (5)   | 0.124 (5)   | 0.117 (5)   | 0.035 (4)    | -0.001 (4)  | 0.017 (4)    |
| O4  | 0.163 (4)   | 0.074 (2)   | 0.126 (3)   | 0.015 (3)    | 0.029 (3)   | 0.034 (2)    |
| C11 | 0.178 (6)   | 0.129 (5)   | 0.093 (4)   | 0.006 (5)    | 0.077 (4)   | -0.016 (4)   |
| O16 | 0.091 (3)   | 0.351 (8)   | 0.093 (3)   | 0.072 (4)    | 0.030 (2)   | 0.078 (4)    |

## supplementary materials

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|     |             |           |             |              |             |              |
|-----|-------------|-----------|-------------|--------------|-------------|--------------|
| O10 | 0.0792 (19) | 0.093 (2) | 0.0483 (15) | -0.0069 (16) | 0.0229 (14) | -0.0034 (14) |
| C51 | 0.073 (2)   | 0.048 (2) | 0.050 (2)   | 0.0057 (18)  | 0.0248 (18) | 0.0122 (16)  |
| C55 | 0.074 (3)   | 0.065 (2) | 0.048 (2)   | 0.011 (2)    | 0.0276 (19) | 0.0118 (17)  |
| O15 | 0.084 (2)   | 0.146 (4) | 0.134 (3)   | 0.000 (2)    | 0.055 (2)   | 0.036 (3)    |
| O11 | 0.091 (2)   | 0.091 (2) | 0.0687 (18) | 0.0056 (17)  | 0.0435 (17) | 0.0024 (16)  |
| C52 | 0.072 (2)   | 0.056 (2) | 0.052 (2)   | 0.0022 (18)  | 0.0310 (18) | 0.0086 (16)  |
| C56 | 0.060 (2)   | 0.065 (2) | 0.052 (2)   | 0.0084 (18)  | 0.0239 (17) | 0.0137 (17)  |
| N12 | 0.077 (2)   | 0.081 (2) | 0.068 (2)   | -0.007 (2)   | 0.0335 (19) | 0.0014 (19)  |
| N13 | 0.092 (3)   | 0.082 (3) | 0.050 (2)   | -0.003 (2)   | 0.015 (2)   | 0.0058 (17)  |
| C54 | 0.077 (3)   | 0.054 (2) | 0.0451 (19) | 0.0025 (19)  | 0.0174 (18) | 0.0067 (16)  |
| C53 | 0.070 (3)   | 0.057 (2) | 0.061 (2)   | -0.0025 (19) | 0.022 (2)   | 0.0076 (18)  |
| O14 | 0.118 (3)   | 0.139 (3) | 0.0493 (17) | 0.002 (2)    | 0.0315 (18) | -0.0001 (18) |
| N14 | 0.075 (3)   | 0.133 (4) | 0.058 (2)   | 0.019 (2)    | 0.028 (2)   | 0.014 (2)    |
| O12 | 0.110 (3)   | 0.194 (4) | 0.108 (3)   | -0.066 (3)   | 0.068 (2)   | -0.041 (3)   |
| O13 | 0.091 (3)   | 0.147 (3) | 0.067 (2)   | -0.023 (2)   | 0.0081 (18) | -0.005 (2)   |
| C59 | 0.080 (3)   | 0.095 (3) | 0.072 (3)   | 0.011 (3)    | 0.019 (3)   | 0.021 (3)    |
| O17 | 0.104 (3)   | 0.151 (4) | 0.084 (2)   | 0.012 (3)    | -0.012 (2)  | 0.039 (2)    |
| N15 | 0.072 (2)   | 0.085 (3) | 0.064 (2)   | 0.0166 (19)  | 0.0122 (17) | 0.0171 (18)  |
| C58 | 0.092 (4)   | 0.133 (5) | 0.078 (3)   | 0.038 (3)    | 0.004 (3)   | 0.018 (3)    |
| C57 | 0.105 (4)   | 0.101 (4) | 0.115 (4)   | 0.004 (3)    | 0.041 (3)   | 0.026 (3)    |
| C33 | 0.129 (6)   | 0.127 (5) | 0.119 (5)   | 0.007 (4)    | -0.013 (4)  | 0.018 (4)    |
| C44 | 0.251 (11)  | 0.190 (7) | 0.152 (7)   | -0.007 (9)   | 0.096 (7)   | -0.059 (7)   |
| C43 | 0.139 (6)   | 0.214 (7) | 0.111 (5)   | 0.028 (6)    | 0.072 (5)   | -0.026 (6)   |

### *Geometric parameters (Å, °)*

|        |           |          |           |
|--------|-----------|----------|-----------|
| Cd1—N5 | 2.233 (2) | C8—C7    | 1.384 (6) |
| Cd1—N1 | 2.242 (3) | C6—C7    | 1.366 (7) |
| Cd1—N3 | 2.250 (3) | C6—H6    | 0.9300    |
| Cd1—N7 | 2.263 (3) | C27—C28  | 1.396 (6) |
| Cd1—O2 | 2.561 (2) | C27—H27  | 0.9300    |
| Cd1—O1 | 2.618 (2) | C37—C38  | 1.377 (5) |
| O1—C1  | 1.414 (4) | C37—H37  | 0.9300    |
| O1—C12 | 1.416 (4) | C31—C32  | 1.500 (6) |
| O2—C23 | 1.416 (4) | C31—H31A | 0.9700    |
| O2—C34 | 1.412 (4) | C31—H31B | 0.9700    |
| N5—C24 | 1.321 (4) | C48—N10  | 1.447 (5) |
| N5—C25 | 1.391 (4) | C28—C29  | 1.372 (6) |
| N4—C13 | 1.353 (4) | C28—H28  | 0.9300    |
| N4—C19 | 1.386 (4) | C29—H29  | 0.9300    |
| N4—C20 | 1.462 (4) | C45—C50  | 1.445 (5) |
| N3—C13 | 1.314 (4) | C10—C11  | 1.516 (7) |
| N3—C14 | 1.394 (4) | C10—H10A | 0.9700    |
| N1—C2  | 1.319 (4) | C10—H10B | 0.9700    |
| N1—C3  | 1.390 (4) | C7—H7    | 0.9300    |
| N7—C35 | 1.316 (4) | C1—H1A   | 0.9700    |
| N7—C36 | 1.388 (4) | C1—H1B   | 0.9700    |
| N6—C24 | 1.353 (4) | C4—H4    | 0.9300    |
| N6—C30 | 1.382 (4) | O6—N10   | 1.230 (5) |

|          |           |          |            |
|----------|-----------|----------|------------|
| N6—C31   | 1.481 (4) | N11—O9   | 1.188 (6)  |
| N8—C35   | 1.354 (4) | N11—O8   | 1.213 (6)  |
| N8—C41   | 1.383 (4) | N11—C50  | 1.454 (6)  |
| N8—C42   | 1.464 (5) | C39—C38  | 1.379 (6)  |
| C24—C23  | 1.485 (4) | C39—H39  | 0.9300     |
| C13—C12  | 1.488 (4) | C42—C43  | 1.445 (7)  |
| C14—C15  | 1.388 (4) | C42—H42A | 0.9700     |
| C14—C19  | 1.385 (4) | C42—H42B | 0.9700     |
| C23—H23A | 0.9700    | C21—C22  | 1.4995 (7) |
| C23—H23B | 0.9700    | C21—H21A | 0.9700     |
| C19—C18  | 1.390 (4) | C21—H21B | 0.9700     |
| C25—C26  | 1.388 (5) | C32—C33  | 1.456 (8)  |
| C25—C30  | 1.392 (4) | C32—H32A | 0.9700     |
| C35—C34  | 1.490 (4) | C32—H32B | 0.9700     |
| C12—H12A | 0.9700    | C38—H38  | 0.9300     |
| C12—H12B | 0.9700    | C22—H22A | 0.9600     |
| C40—C39  | 1.372 (6) | C22—H22B | 0.9600     |
| C40—C41  | 1.395 (5) | C22—H22C | 0.9600     |
| C40—H40  | 0.9300    | C11—H11A | 0.9600     |
| C30—C29  | 1.385 (5) | C11—H11B | 0.9600     |
| C34—H34A | 0.9700    | C11—H11C | 0.9600     |
| C34—H34B | 0.9700    | O16—N14  | 1.206 (5)  |
| C36—C41  | 1.387 (5) | O10—C51  | 1.232 (4)  |
| C36—C37  | 1.392 (5) | C51—C52  | 1.438 (5)  |
| C9—N2    | 1.483 (5) | C51—C56  | 1.445 (5)  |
| C9—C10   | 1.507 (7) | C55—C56  | 1.357 (5)  |
| C9—H9A   | 0.9700    | C55—C54  | 1.374 (5)  |
| C9—H9B   | 0.9700    | C55—H55  | 0.9300     |
| C18—C17  | 1.364 (5) | O15—N14  | 1.192 (5)  |
| C18—H18  | 0.9300    | O11—N12  | 1.215 (4)  |
| C3—C4    | 1.373 (5) | C52—C53  | 1.369 (5)  |
| C3—C8    | 1.393 (5) | C52—N12  | 1.445 (5)  |
| C15—C16  | 1.368 (5) | C56—N14  | 1.452 (5)  |
| C15—H15  | 0.9300    | N12—O12  | 1.215 (5)  |
| C26—C27  | 1.371 (5) | N13—O14  | 1.217 (5)  |
| C26—H26  | 0.9300    | N13—O13  | 1.224 (5)  |
| N2—C2    | 1.345 (4) | N13—C54  | 1.438 (5)  |
| N2—C8    | 1.377 (5) | C54—C53  | 1.377 (5)  |
| C2—C1    | 1.479 (5) | C53—H53  | 0.9300     |
| O7—N10   | 1.216 (5) | C59—O17  | 1.209 (5)  |
| C20—C21  | 1.461 (6) | C59—N15  | 1.307 (5)  |
| C20—H20A | 0.9700    | C59—H59  | 0.9300     |
| C20—H20B | 0.9700    | N15—C57  | 1.432 (6)  |
| O3—C45   | 1.235 (4) | N15—C58  | 1.451 (5)  |
| C5—C6    | 1.386 (7) | C58—H58A | 0.9600     |
| C5—C4    | 1.382 (6) | C58—H58B | 0.9600     |
| C5—H5    | 0.9300    | C58—H58C | 0.9600     |
| C46—C47  | 1.346 (5) | C57—H57A | 0.9600     |
| C46—C45  | 1.440 (5) | C57—H57B | 0.9600     |

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| C46—N9     | 1.471 (5)   | C57—H57C      | 0.9600     |
| C16—C17    | 1.396 (5)   | C33—H33A      | 0.9600     |
| C16—H16    | 0.9300      | C33—H33B      | 0.9600     |
| C47—C48    | 1.376 (5)   | C33—H33C      | 0.9600     |
| C47—H47    | 0.9300      | C44—C43       | 1.4997 (9) |
| N9—O5      | 1.133 (5)   | C44—H44A      | 0.9600     |
| N9—O4      | 1.204 (5)   | C44—H44B      | 0.9600     |
| C49—C48    | 1.374 (6)   | C44—H44C      | 0.9600     |
| C49—C50    | 1.374 (6)   | C43—H43A      | 0.9700     |
| C49—H49    | 0.9300      | C43—H43B      | 0.9700     |
| C17—H17    | 0.9300      |               |            |
| N5—Cd1—N1  | 102.14 (9)  | C28—C27—H27   | 119.6      |
| N5—Cd1—N3  | 108.82 (9)  | C38—C37—C36   | 116.4 (4)  |
| N1—Cd1—N3  | 127.24 (9)  | C38—C37—H37   | 121.8      |
| N5—Cd1—N7  | 131.02 (9)  | C36—C37—H37   | 121.8      |
| N1—Cd1—N7  | 101.21 (9)  | N6—C31—C32    | 114.9 (3)  |
| N3—Cd1—N7  | 89.53 (9)   | N6—C31—H31A   | 108.5      |
| N5—Cd1—O2  | 65.77 (8)   | C32—C31—H31A  | 108.5      |
| N1—Cd1—O2  | 115.93 (10) | N6—C31—H31B   | 108.5      |
| N3—Cd1—O2  | 115.47 (9)  | C32—C31—H31B  | 108.5      |
| N7—Cd1—O2  | 65.34 (8)   | H31A—C31—H31B | 107.5      |
| N5—Cd1—O1  | 107.15 (9)  | C49—C48—C47   | 120.8 (4)  |
| N1—Cd1—O1  | 65.86 (9)   | C49—C48—N10   | 119.9 (4)  |
| N3—Cd1—O1  | 64.71 (8)   | C47—C48—N10   | 119.3 (4)  |
| N7—Cd1—O1  | 121.64 (8)  | C29—C28—C27   | 122.2 (4)  |
| O2—Cd1—O1  | 172.80 (7)  | C29—C28—H28   | 118.9      |
| C1—O1—C12  | 115.2 (2)   | C27—C28—H28   | 118.9      |
| C1—O1—Cd1  | 117.3 (2)   | C28—C29—C30   | 116.9 (3)  |
| C12—O1—Cd1 | 116.95 (17) | C28—C29—H29   | 121.6      |
| C23—O2—C34 | 115.5 (2)   | C30—C29—H29   | 121.6      |
| C23—O2—Cd1 | 117.99 (18) | O3—C45—C46    | 121.8 (4)  |
| C34—O2—Cd1 | 119.18 (18) | O3—C45—C50    | 127.5 (4)  |
| C24—N5—C25 | 105.9 (2)   | C46—C45—C50   | 110.7 (3)  |
| C24—N5—Cd1 | 124.2 (2)   | C9—C10—C11    | 111.9 (5)  |
| C25—N5—Cd1 | 129.8 (2)   | C9—C10—H10A   | 109.2      |
| C13—N4—C19 | 107.2 (2)   | C11—C10—H10A  | 109.2      |
| C13—N4—C20 | 126.9 (3)   | C9—C10—H10B   | 109.2      |
| C19—N4—C20 | 125.8 (3)   | C11—C10—H10B  | 109.2      |
| C13—N3—C14 | 105.9 (2)   | H10A—C10—H10B | 107.9      |
| C13—N3—Cd1 | 124.8 (2)   | C6—C7—C8      | 117.0 (5)  |
| C14—N3—Cd1 | 127.45 (19) | C6—C7—H7      | 121.5      |
| C2—N1—C3   | 106.2 (3)   | C8—C7—H7      | 121.5      |
| C2—N1—Cd1  | 124.9 (2)   | O1—C1—C2      | 107.2 (3)  |
| C3—N1—Cd1  | 128.6 (2)   | O1—C1—H1A     | 110.3      |
| C35—N7—C36 | 105.6 (3)   | C2—C1—H1A     | 110.3      |
| C35—N7—Cd1 | 124.2 (2)   | O1—C1—H1B     | 110.3      |
| C36—N7—Cd1 | 129.3 (2)   | C2—C1—H1B     | 110.3      |
| C24—N6—C30 | 106.8 (3)   | H1A—C1—H1B    | 108.5      |
| C24—N6—C31 | 126.3 (3)   | C3—C4—C5      | 117.4 (4)  |

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| C30—N6—C31    | 126.8 (3) | C3—C4—H4      | 121.3     |
| C35—N8—C41    | 106.8 (3) | C5—C4—H4      | 121.3     |
| C35—N8—C42    | 126.4 (3) | O9—N11—O8     | 121.5 (5) |
| C41—N8—C42    | 126.8 (3) | O9—N11—C50    | 120.8 (5) |
| N5—C24—N6     | 112.4 (3) | O8—N11—C50    | 117.7 (5) |
| N5—C24—C23    | 123.7 (3) | C40—C39—C38   | 121.6 (4) |
| N6—C24—C23    | 123.8 (3) | C40—C39—H39   | 119.2     |
| N3—C13—N4     | 112.2 (3) | C38—C39—H39   | 119.2     |
| N3—C13—C12    | 123.8 (3) | C49—C50—N11   | 118.0 (4) |
| N4—C13—C12    | 124.1 (3) | C49—C50—C45   | 123.6 (4) |
| C15—C14—C19   | 120.8 (3) | N11—C50—C45   | 118.5 (4) |
| C15—C14—N3    | 130.2 (3) | O7—N10—O6     | 123.8 (4) |
| C19—C14—N3    | 109.0 (3) | O7—N10—C48    | 118.4 (5) |
| O2—C23—C24    | 105.4 (2) | O6—N10—C48    | 117.8 (4) |
| O2—C23—H23A   | 110.7     | N8—C42—C43    | 117.0 (4) |
| C24—C23—H23A  | 110.7     | N8—C42—H42A   | 108.0     |
| O2—C23—H23B   | 110.7     | C43—C42—H42A  | 108.0     |
| C24—C23—H23B  | 110.7     | N8—C42—H42B   | 108.0     |
| H23A—C23—H23B | 108.8     | C43—C42—H42B  | 108.0     |
| N4—C19—C14    | 105.7 (3) | H42A—C42—H42B | 107.3     |
| N4—C19—C18    | 132.5 (3) | C22—C21—C20   | 111.3 (4) |
| C14—C19—C18   | 121.7 (3) | C22—C21—H21A  | 109.4     |
| C26—C25—N5    | 130.4 (3) | C20—C21—H21A  | 109.4     |
| C26—C25—C30   | 121.1 (3) | C22—C21—H21B  | 109.4     |
| N5—C25—C30    | 108.5 (3) | C20—C21—H21B  | 109.4     |
| N7—C35—N8     | 112.6 (3) | H21A—C21—H21B | 108.0     |
| N7—C35—C34    | 123.5 (3) | C33—C32—C31   | 114.9 (6) |
| N8—C35—C34    | 123.9 (3) | C33—C32—H32A  | 108.5     |
| O1—C12—C13    | 106.0 (2) | C31—C32—H32A  | 108.5     |
| O1—C12—H12A   | 110.5     | C33—C32—H32B  | 108.5     |
| C13—C12—H12A  | 110.5     | C31—C32—H32B  | 108.5     |
| O1—C12—H12B   | 110.5     | H32A—C32—H32B | 107.5     |
| C13—C12—H12B  | 110.5     | C37—C38—C39   | 122.6 (4) |
| H12A—C12—H12B | 108.7     | C37—C38—H38   | 118.7     |
| C39—C40—C41   | 116.6 (4) | C39—C38—H38   | 118.7     |
| C39—C40—H40   | 121.7     | C21—C22—H22A  | 109.5     |
| C41—C40—H40   | 121.7     | C21—C22—H22B  | 109.5     |
| N6—C30—C29    | 132.3 (3) | H22A—C22—H22B | 109.5     |
| N6—C30—C25    | 106.3 (3) | C21—C22—H22C  | 109.5     |
| C29—C30—C25   | 121.3 (3) | H22A—C22—H22C | 109.5     |
| O2—C34—C35    | 105.8 (2) | H22B—C22—H22C | 109.5     |
| O2—C34—H34A   | 110.6     | C10—C11—H11A  | 109.5     |
| C35—C34—H34A  | 110.6     | C10—C11—H11B  | 109.5     |
| O2—C34—H34B   | 110.6     | H11A—C11—H11B | 109.5     |
| C35—C34—H34B  | 110.6     | C10—C11—H11C  | 109.5     |
| H34A—C34—H34B | 108.7     | H11A—C11—H11C | 109.5     |
| N7—C36—C41    | 109.1 (3) | H11B—C11—H11C | 109.5     |
| N7—C36—C37    | 129.8 (3) | O10—C51—C52   | 126.5 (3) |
| C41—C36—C37   | 121.1 (3) | O10—C51—C56   | 122.2 (4) |

## supplementary materials

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| N2—C9—C10     | 112.7 (4) | C52—C51—C56   | 111.3 (3) |
| N2—C9—H9A     | 109.1     | C56—C55—C54   | 119.0 (4) |
| C10—C9—H9A    | 109.1     | C56—C55—H55   | 120.5     |
| N2—C9—H9B     | 109.1     | C54—C55—H55   | 120.5     |
| C10—C9—H9B    | 109.1     | C53—C52—C51   | 123.6 (3) |
| H9A—C9—H9B    | 107.8     | C53—C52—N12   | 116.6 (4) |
| C17—C18—C19   | 116.7 (3) | C51—C52—N12   | 119.8 (3) |
| C17—C18—H18   | 121.6     | C55—C56—C51   | 125.2 (4) |
| C19—C18—H18   | 121.6     | C55—C56—N14   | 117.2 (3) |
| C4—C3—N1      | 130.5 (3) | C51—C56—N14   | 117.5 (3) |
| C4—C3—C8      | 121.3 (4) | O12—N12—O11   | 121.7 (4) |
| N1—C3—C8      | 108.1 (3) | O12—N12—C52   | 118.4 (4) |
| C16—C15—C14   | 117.7 (3) | O11—N12—C52   | 119.9 (3) |
| C16—C15—H15   | 121.2     | O14—N13—O13   | 123.7 (4) |
| C14—C15—H15   | 121.2     | O14—N13—C54   | 118.1 (4) |
| N8—C41—C36    | 105.9 (3) | O13—N13—C54   | 118.1 (4) |
| N8—C41—C40    | 132.4 (4) | C55—C54—C53   | 120.4 (3) |
| C36—C41—C40   | 121.7 (4) | C55—C54—N13   | 119.9 (4) |
| C27—C26—C25   | 117.6 (3) | C53—C54—N13   | 119.7 (4) |
| C27—C26—H26   | 121.2     | C52—C53—C54   | 120.2 (4) |
| C25—C26—H26   | 121.2     | C52—C53—H53   | 119.9     |
| C2—N2—C8      | 107.2 (3) | C54—C53—H53   | 119.9     |
| C2—N2—C9      | 126.9 (4) | O15—N14—O16   | 122.6 (5) |
| C8—N2—C9      | 125.9 (3) | O15—N14—C56   | 119.8 (4) |
| N1—C2—N2      | 112.2 (3) | O16—N14—C56   | 117.4 (4) |
| N1—C2—C1      | 124.6 (3) | O17—C59—N15   | 124.0 (5) |
| N2—C2—C1      | 123.2 (3) | O17—C59—H59   | 118.0     |
| N4—C20—C21    | 115.2 (3) | N15—C59—H59   | 118.0     |
| N4—C20—H20A   | 108.5     | C59—N15—C57   | 122.4 (4) |
| C21—C20—H20A  | 108.5     | C59—N15—C58   | 118.7 (4) |
| N4—C20—H20B   | 108.5     | C57—N15—C58   | 118.7 (4) |
| C21—C20—H20B  | 108.5     | N15—C58—H58A  | 109.5     |
| H20A—C20—H20B | 107.5     | N15—C58—H58B  | 109.5     |
| C6—C5—C4      | 121.0 (5) | H58A—C58—H58B | 109.5     |
| C6—C5—H5      | 119.5     | N15—C58—H58C  | 109.5     |
| C4—C5—H5      | 119.5     | H58A—C58—H58C | 109.5     |
| C47—C46—C45   | 126.4 (4) | H58B—C58—H58C | 109.5     |
| C47—C46—N9    | 118.3 (3) | N15—C57—H57A  | 109.5     |
| C45—C46—N9    | 115.3 (3) | N15—C57—H57B  | 109.5     |
| C15—C16—C17   | 121.0 (3) | H57A—C57—H57B | 109.5     |
| C15—C16—H16   | 119.5     | N15—C57—H57C  | 109.5     |
| C17—C16—H16   | 119.5     | H57A—C57—H57C | 109.5     |
| C46—C47—C48   | 118.5 (4) | H57B—C57—H57C | 109.5     |
| C46—C47—H47   | 120.8     | C32—C33—H33A  | 109.5     |
| C48—C47—H47   | 120.8     | C32—C33—H33B  | 109.5     |
| O5—N9—O4      | 122.0 (4) | H33A—C33—H33B | 109.5     |
| O5—N9—C46     | 121.0 (4) | C32—C33—H33C  | 109.5     |
| O4—N9—C46     | 117.0 (4) | H33A—C33—H33C | 109.5     |
| C48—C49—C50   | 119.9 (4) | H33B—C33—H33C | 109.5     |

|               |            |                 |            |
|---------------|------------|-----------------|------------|
| C48—C49—H49   | 120.1      | C43—C44—H44A    | 109.5      |
| C50—C49—H49   | 120.1      | C43—C44—H44B    | 109.5      |
| C18—C17—C16   | 122.1 (3)  | H44A—C44—H44B   | 109.5      |
| C18—C17—H17   | 119.0      | C43—C44—H44C    | 109.5      |
| C16—C17—H17   | 119.0      | H44A—C44—H44C   | 109.5      |
| N2—C8—C7      | 132.5 (4)  | H44B—C44—H44C   | 109.5      |
| N2—C8—C3      | 106.3 (3)  | C44—C43—C42     | 114.7 (6)  |
| C7—C8—C3      | 121.2 (5)  | C44—C43—H43A    | 108.6      |
| C7—C6—C5      | 122.1 (5)  | C42—C43—H43A    | 108.6      |
| C7—C6—H6      | 118.9      | C44—C43—H43B    | 108.6      |
| C5—C6—H6      | 118.9      | C42—C43—H43B    | 108.6      |
| C26—C27—C28   | 120.9 (4)  | H43A—C43—H43B   | 107.6      |
| C26—C27—H27   | 119.6      |                 |            |
| N5—Cd1—O1—C1  | -96.2 (2)  | Cd1—N1—C3—C4    | 7.0 (5)    |
| N1—Cd1—O1—C1  | -0.3 (2)   | C2—N1—C3—C8     | 0.2 (4)    |
| N3—Cd1—O1—C1  | 160.6 (3)  | Cd1—N1—C3—C8    | -173.5 (2) |
| N7—Cd1—O1—C1  | 88.2 (2)   | C19—C14—C15—C16 | 0.2 (5)    |
| O2—Cd1—O1—C1  | -106.3 (6) | N3—C14—C15—C16  | -178.1 (3) |
| N5—Cd1—O1—C12 | 120.6 (2)  | C35—N8—C41—C36  | -0.5 (3)   |
| N1—Cd1—O1—C12 | -143.5 (2) | C42—N8—C41—C36  | 178.7 (3)  |
| N3—Cd1—O1—C12 | 17.4 (2)   | C35—N8—C41—C40  | 178.9 (4)  |
| N7—Cd1—O1—C12 | -55.0 (2)  | C42—N8—C41—C40  | -1.8 (6)   |
| O2—Cd1—O1—C12 | 110.5 (6)  | N7—C36—C41—N8   | -0.1 (4)   |
| N5—Cd1—O2—C23 | -15.5 (2)  | C37—C36—C41—N8  | 179.6 (3)  |
| N1—Cd1—O2—C23 | -107.6 (2) | N7—C36—C41—C40  | -179.7 (3) |
| N3—Cd1—O2—C23 | 84.7 (2)   | C37—C36—C41—C40 | 0.0 (5)    |
| N7—Cd1—O2—C23 | 161.5 (2)  | C39—C40—C41—N8  | 180.0 (4)  |
| O1—Cd1—O2—C23 | -4.9 (7)   | C39—C40—C41—C36 | -0.6 (5)   |
| N5—Cd1—O2—C34 | -164.2 (3) | N5—C25—C26—C27  | 178.6 (3)  |
| N1—Cd1—O2—C34 | 103.7 (2)  | C30—C25—C26—C27 | 0.7 (5)    |
| N3—Cd1—O2—C34 | -64.0 (2)  | C10—C9—N2—C2    | -103.1 (5) |
| N7—Cd1—O2—C34 | 12.8 (2)   | C10—C9—N2—C8    | 75.9 (6)   |
| O1—Cd1—O2—C34 | -153.7 (5) | C3—N1—C2—N2     | -0.3 (4)   |
| N1—Cd1—N5—C24 | 123.1 (2)  | Cd1—N1—C2—N2    | 173.7 (2)  |
| N3—Cd1—N5—C24 | -100.2 (2) | C3—N1—C2—C1     | -179.6 (3) |
| N7—Cd1—N5—C24 | 6.3 (3)    | Cd1—N1—C2—C1    | -5.6 (5)   |
| O2—Cd1—N5—C24 | 9.9 (2)    | C8—N2—C2—N1     | 0.3 (4)    |
| O1—Cd1—N5—C24 | -168.7 (2) | C9—N2—C2—N1     | 179.5 (4)  |
| N1—Cd1—N5—C25 | -59.3 (3)  | C8—N2—C2—C1     | 179.6 (3)  |
| N3—Cd1—N5—C25 | 77.3 (3)   | C9—N2—C2—C1     | -1.2 (6)   |
| N7—Cd1—N5—C25 | -176.1 (2) | C13—N4—C20—C21  | -113.5 (4) |
| O2—Cd1—N5—C25 | -172.5 (3) | C19—N4—C20—C21  | 63.6 (5)   |
| O1—Cd1—N5—C25 | 8.9 (3)    | C14—C15—C16—C17 | 0.6 (5)    |
| N5—Cd1—N3—C13 | -115.9 (2) | C45—C46—C47—C48 | 2.6 (6)    |
| N1—Cd1—N3—C13 | 6.7 (3)    | N9—C46—C47—C48  | -176.2 (3) |
| N7—Cd1—N3—C13 | 110.5 (2)  | C47—C46—N9—O5   | -83.6 (6)  |
| O2—Cd1—N3—C13 | 172.7 (2)  | C45—C46—N9—O5   | 97.4 (5)   |
| O1—Cd1—N3—C13 | -15.3 (2)  | C47—C46—N9—O4   | 97.4 (5)   |
| N5—Cd1—N3—C14 | 81.8 (2)   | C45—C46—N9—O4   | -81.6 (5)  |

## supplementary materials

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|                |              |                 |            |
|----------------|--------------|-----------------|------------|
| N1—Cd1—N3—C14  | -155.6 (2)   | C19—C18—C17—C16 | 0.9 (5)    |
| N7—Cd1—N3—C14  | -51.8 (2)    | C15—C16—C17—C18 | -1.2 (6)   |
| O2—Cd1—N3—C14  | 10.4 (3)     | C2—N2—C8—C7     | -178.2 (4) |
| O1—Cd1—N3—C14  | -177.6 (3)   | C9—N2—C8—C7     | 2.6 (7)    |
| N5—Cd1—N1—C2   | 106.5 (3)    | C2—N2—C8—C3     | -0.2 (4)   |
| N3—Cd1—N1—C2   | -18.8 (3)    | C9—N2—C8—C3     | -179.4 (4) |
| N7—Cd1—N1—C2   | -116.9 (3)   | C4—C3—C8—N2     | 179.5 (3)  |
| O2—Cd1—N1—C2   | 175.2 (2)    | N1—C3—C8—N2     | 0.0 (4)    |
| O1—Cd1—N1—C2   | 2.9 (2)      | C4—C3—C8—C7     | -2.2 (6)   |
| N5—Cd1—N1—C3   | -80.9 (3)    | N1—C3—C8—C7     | 178.3 (4)  |
| N3—Cd1—N1—C3   | 153.8 (2)    | C4—C5—C6—C7     | -0.7 (8)   |
| N7—Cd1—N1—C3   | 55.7 (3)     | C25—C26—C27—C28 | 0.0 (5)    |
| O2—Cd1—N1—C3   | -12.1 (3)    | N7—C36—C37—C38  | 179.9 (3)  |
| O1—Cd1—N1—C3   | 175.6 (3)    | C41—C36—C37—C38 | 0.3 (5)    |
| N5—Cd1—N7—C35  | -6.6 (3)     | C24—N6—C31—C32  | 82.8 (5)   |
| N1—Cd1—N7—C35  | -123.8 (2)   | C30—N6—C31—C32  | -101.1 (5) |
| N3—Cd1—N7—C35  | 108.3 (3)    | C50—C49—C48—C47 | -1.8 (6)   |
| O2—Cd1—N7—C35  | -10.2 (2)    | C50—C49—C48—N10 | 176.6 (3)  |
| O1—Cd1—N7—C35  | 167.8 (2)    | C46—C47—C48—C49 | 0.5 (6)    |
| N5—Cd1—N7—C36  | -174.0 (2)   | C46—C47—C48—N10 | -178.0 (3) |
| N1—Cd1—N7—C36  | 68.9 (3)     | C26—C27—C28—C29 | -0.5 (6)   |
| N3—Cd1—N7—C36  | -59.1 (3)    | C27—C28—C29—C30 | 0.3 (6)    |
| O2—Cd1—N7—C36  | -177.6 (3)   | N6—C30—C29—C28  | -177.6 (4) |
| O1—Cd1—N7—C36  | 0.4 (3)      | C25—C30—C29—C28 | 0.4 (5)    |
| C25—N5—C24—N6  | -1.1 (3)     | C47—C46—C45—O3  | 176.9 (4)  |
| Cd1—N5—C24—N6  | 176.98 (19)  | N9—C46—C45—O3   | -4.2 (5)   |
| C25—N5—C24—C23 | 177.6 (3)    | C47—C46—C45—C50 | -3.8 (5)   |
| Cd1—N5—C24—C23 | -4.4 (4)     | N9—C46—C45—C50  | 175.1 (3)  |
| C30—N6—C24—N5  | 0.6 (3)      | N2—C9—C10—C11   | 177.2 (5)  |
| C31—N6—C24—N5  | 177.3 (3)    | C5—C6—C7—C8     | -0.9 (8)   |
| C30—N6—C24—C23 | -178.0 (3)   | N2—C8—C7—C6     | -180.0 (5) |
| C31—N6—C24—C23 | -1.3 (5)     | C3—C8—C7—C6     | 2.3 (7)    |
| C14—N3—C13—N4  | -0.6 (3)     | C12—O1—C1—C2    | 142.1 (3)  |
| Cd1—N3—C13—N4  | -166.06 (18) | Cd1—O1—C1—C2    | -1.7 (4)   |
| C14—N3—C13—C12 | 178.4 (3)    | N1—C2—C1—O1     | 4.5 (5)    |
| Cd1—N3—C13—C12 | 12.9 (4)     | N2—C2—C1—O1     | -174.7 (3) |
| C19—N4—C13—N3  | 0.6 (3)      | N1—C3—C4—C5     | 179.9 (3)  |
| C20—N4—C13—N3  | 178.2 (3)    | C8—C3—C4—C5     | 0.6 (5)    |
| C19—N4—C13—C12 | -178.4 (3)   | C6—C5—C4—C3     | 0.9 (6)    |
| C20—N4—C13—C12 | -0.8 (5)     | C41—C40—C39—C38 | 0.9 (6)    |
| C13—N3—C14—C15 | 178.9 (3)    | C48—C49—C50—N11 | -179.0 (4) |
| Cd1—N3—C14—C15 | -16.2 (5)    | C48—C49—C50—C45 | 0.3 (6)    |
| C13—N3—C14—C19 | 0.4 (3)      | O9—N11—C50—C49  | 156.4 (5)  |
| Cd1—N3—C14—C19 | 165.3 (2)    | O8—N11—C50—C49  | -24.1 (6)  |
| C34—O2—C23—C24 | 167.1 (3)    | O9—N11—C50—C45  | -22.9 (7)  |
| Cd1—O2—C23—C24 | 17.3 (3)     | O8—N11—C50—C45  | 156.5 (5)  |
| N5—C24—C23—O2  | -9.7 (4)     | O3—C45—C50—C49  | -178.5 (4) |
| N6—C24—C23—O2  | 168.8 (3)    | C46—C45—C50—C49 | 2.3 (5)    |
| C13—N4—C19—C14 | -0.3 (3)     | O3—C45—C50—N11  | 0.8 (6)    |



|                 |            |                 |            |
|-----------------|------------|-----------------|------------|
| C20—N4—C19—C14  | -177.9 (3) | C46—C45—C50—N11 | -178.5 (3) |
| C13—N4—C19—C18  | -178.2 (3) | C49—C48—N10—O7  | 1.9 (6)    |
| C20—N4—C19—C18  | 4.2 (6)    | C47—C48—N10—O7  | -179.6 (4) |
| C15—C14—C19—N4  | -178.7 (3) | C49—C48—N10—O6  | -177.0 (4) |
| N3—C14—C19—N4   | 0.0 (3)    | C47—C48—N10—O6  | 1.5 (5)    |
| C15—C14—C19—C18 | -0.5 (5)   | C35—N8—C42—C43  | -82.5 (6)  |
| N3—C14—C19—C18  | 178.2 (3)  | C41—N8—C42—C43  | 98.4 (5)   |
| C24—N5—C25—C26  | -177.0 (3) | N4—C20—C21—C22  | 58.3 (6)   |
| Cd1—N5—C25—C26  | 5.1 (5)    | N6—C31—C32—C33  | 66.8 (6)   |
| C24—N5—C25—C30  | 1.1 (3)    | C36—C37—C38—C39 | 0.0 (6)    |
| Cd1—N5—C25—C30  | -176.8 (2) | C40—C39—C38—C37 | -0.6 (7)   |
| C36—N7—C35—N8   | -1.1 (3)   | O10—C51—C52—C53 | 177.8 (4)  |
| Cd1—N7—C35—N8   | -171.0 (2) | C56—C51—C52—C53 | -2.4 (5)   |
| C36—N7—C35—C34  | 177.5 (3)  | O10—C51—C52—N12 | -3.9 (6)   |
| Cd1—N7—C35—C34  | 7.7 (4)    | C56—C51—C52—N12 | 175.9 (3)  |
| C41—N8—C35—N7   | 1.1 (4)    | C54—C55—C56—C51 | -2.6 (6)   |
| C42—N8—C35—N7   | -178.2 (3) | C54—C55—C56—N14 | 178.6 (4)  |
| C41—N8—C35—C34  | -177.6 (3) | O10—C51—C56—C55 | -176.2 (4) |
| C42—N8—C35—C34  | 3.1 (5)    | C52—C51—C56—C55 | 4.0 (5)    |
| C1—O1—C12—C13   | -160.5 (3) | O10—C51—C56—N14 | 2.6 (6)    |
| Cd1—O1—C12—C13  | -16.6 (3)  | C52—C51—C56—N14 | -177.2 (4) |
| N3—C13—C12—O1   | 4.6 (4)    | C53—C52—N12—O12 | 19.6 (6)   |
| N4—C13—C12—O1   | -176.5 (3) | C51—C52—N12—O12 | -158.7 (5) |
| C24—N6—C30—C29  | 178.4 (4)  | C53—C52—N12—O11 | -160.5 (4) |
| C31—N6—C30—C29  | 1.7 (6)    | C51—C52—N12—O11 | 21.1 (6)   |
| C24—N6—C30—C25  | 0.1 (3)    | C56—C55—C54—C53 | -0.7 (6)   |
| C31—N6—C30—C25  | -176.6 (3) | C56—C55—C54—N13 | -179.8 (4) |
| C26—C25—C30—N6  | 177.6 (3)  | O14—N13—C54—C55 | -0.1 (6)   |
| N5—C25—C30—N6   | -0.7 (3)   | O13—N13—C54—C55 | 179.0 (4)  |
| C26—C25—C30—C29 | -0.9 (5)   | O14—N13—C54—C53 | -179.3 (4) |
| N5—C25—C30—C29  | -179.2 (3) | O13—N13—C54—C53 | -0.1 (6)   |
| C23—O2—C34—C35  | -162.3 (3) | C51—C52—C53—C54 | -0.5 (6)   |
| Cd1—O2—C34—C35  | -12.8 (3)  | N12—C52—C53—C54 | -178.8 (4) |
| N7—C35—C34—O2   | 4.5 (4)    | C55—C54—C53—C52 | 2.2 (6)    |
| N8—C35—C34—O2   | -177.0 (3) | N13—C54—C53—C52 | -178.7 (4) |
| C35—N7—C36—C41  | 0.7 (3)    | C55—C56—N14—O15 | 43.0 (6)   |
| Cd1—N7—C36—C41  | 169.9 (2)  | C51—C56—N14—O15 | -135.9 (5) |
| C35—N7—C36—C37  | -178.9 (3) | C55—C56—N14—O16 | -132.0 (5) |
| Cd1—N7—C36—C37  | -9.7 (5)   | C51—C56—N14—O16 | 49.1 (6)   |
| N4—C19—C18—C17  | 177.6 (3)  | O17—C59—N15—C57 | -2.7 (8)   |
| C14—C19—C18—C17 | -0.1 (5)   | O17—C59—N15—C58 | -178.8 (5) |
| C2—N1—C3—C4     | -179.3 (4) | N8—C42—C43—C44  | -54.4 (9)  |

Fig. 1

