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# Bis[bis(1-ethylbenzimidazol-2-ylmethyl) ether]cobalt(II) dipicrate dimethylformamide disolvate

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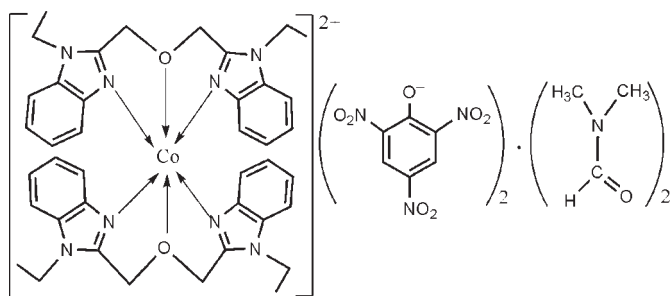
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Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å; disorder in main residue;  $R$  factor = 0.042;  $wR$  factor = 0.136; data-to-parameter ratio = 13.1.

In the title complex,  $[\text{Co}(\text{C}_{20}\text{H}_{22}\text{N}_4\text{O}_2)_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot 2\text{C}_3\text{H}_7\text{NO}$ , the  $\text{Co}^{\text{II}}$  ion is coordinated by two sets of two N atoms and an O atom from two independent tridentate ligands in a distorted octahedral coordination environment. There are significant differences between chemically equivalent coordination bond lengths. The crystal structure is stabilized by weak intermolecular  $\text{C}-\text{H} \cdots \text{O}$  hydrogen bonds and weak  $\pi-\pi$  stacking interactions [centroid-centroid distance 3.495 (1) Å]. In one of the anions one nitro group is rotationally disordered about the  $\text{C}-\text{N}$  bond with refined occupancies of 0.524 (8) and 0.476 (8).

## Related literature

For related structures, see: Wu, Yun, Huang *et al.* (2009); Wu, Yun, Li *et al.* (2009); Yun *et al.* (2008).



## Experimental

### Crystal data

$[\text{Co}(\text{C}_{20}\text{H}_{22}\text{N}_4\text{O}_2)_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot 2\text{C}_3\text{H}_7\text{NO}$   
 $M_r = 1330.17$   
 Triclinic,  $P\bar{1}$   
 $a = 13.8799$  (4) Å  
 $b = 14.6525$  (4) Å

$c = 16.5701$  (3) Å  
 $\alpha = 110.664$  (1)°  
 $\beta = 96.470$  (1)°  
 $\gamma = 99.612$  (1)°  
 $V = 3054.62$  (13) Å<sup>3</sup>  
 $Z = 2$

Mo  $K\alpha$  radiation  
 $\mu = 0.37$  mm<sup>-1</sup>

$T = 153$  K  
 $0.38 \times 0.22 \times 0.14$  mm

### Data collection

Rigaku R-Axis Spider diffractometer  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\text{min}} = 0.873$ ,  $T_{\text{max}} = 0.950$

24377 measured reflections  
 11225 independent reflections  
 8833 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.136$   
 $S = 1.14$   
 11225 reflections  
 858 parameters

4 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.98$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.90$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

|          |            |          |             |
|----------|------------|----------|-------------|
| Co—N1    | 2.083 (2)  | Co—N5    | 2.174 (2)   |
| Co—N3    | 2.099 (2)  | Co—O2    | 2.1961 (17) |
| Co—N7    | 2.108 (2)  | Co—O1    | 2.2872 (16) |
| N1—Co—N3 | 140.20 (8) | N7—Co—O2 | 73.35 (7)   |
| N1—Co—N7 | 99.60 (8)  | N5—Co—O2 | 72.66 (7)   |
| N3—Co—N7 | 100.49 (8) | N1—Co—O1 | 72.54 (7)   |
| N1—Co—N5 | 97.14 (8)  | N3—Co—O1 | 71.85 (7)   |
| N3—Co—N5 | 85.56 (8)  | N7—Co—O1 | 94.77 (7)   |
| N7—Co—N5 | 144.80 (7) | N5—Co—O1 | 119.81 (7)  |
| N1—Co—O2 | 103.97 (8) | O2—Co—O1 | 167.10 (7)  |
| N3—Co—O2 | 114.58 (7) |          |             |

**Table 2**

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$                       | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|---|--------------|---------------------|--------------|-----------------------|
| C18—H18B <sup>i</sup> ···O12 <sup>i</sup>   | 0.98         | 2.57                | 3.342 (4)    | 135                   |
| C15—H15A <sup>i</sup> ···O13                | 0.95         | 2.56                | 3.191 (3)    | 124                   |
| C18—H18B <sup>i</sup> ···O12 <sup>i</sup>   | 0.98         | 2.57                | 3.342 (4)    | 135                   |
| C28—H28A <sup>i</sup> ···O17 <sup>ii</sup>  | 0.99         | 2.38                | 3.365 (4)    | 173                   |
| C28—H28B <sup>i</sup> ···O10 <sup>iii</sup> | 0.99         | 2.29                | 2.994 (3)    | 128                   |
| C29—H29A <sup>i</sup> ···O14                | 0.99         | 2.39                | 3.331 (3)    | 158                   |
| C35—H35A <sup>i</sup> ···O7 <sup>i</sup>    | 0.95         | 2.44                | 3.158 (3)    | 133                   |
| C53—H53 <sup>i</sup> ···O9 <sup>iv</sup>    | 0.95         | 2.39                | 3.242 (7)    | 148                   |
| C56—H56A <sup>i</sup> ···O3 <sup>v</sup>    | 0.95         | 2.46                | 3.335 (4)    | 154                   |

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

Data collection: *RAPID-AUTO* (Rigaku/MSC 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); 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: LH2889).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m1196-m1197 [ doi:10.1107/S1600536809035934 ]

## Bis[bis(1-ethylbenzimidazol-2-ylmethyl) ether]cobalt(II) dipicrate dimethylformamide disolvate

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### Comment

Interest in bis(2-benzimidazolyl)alkanes and their derivatives are widespread and we have previously reported the crystal structure of some related complexes (Wu, Yun, Huang *et al.*, 2009; Wu, Yun, Li *et al.*, 2009; Yun *et al.*, 2008). The asymmetric unit of the title compound consists of a di[1,3-bis(1-ethylbenzimidazol-2-yl)-2-oxopropane] cobalt(II) cation (Fig. 1), two picrate anions and two molecules of DMF. The Co<sup>II</sup> ion is six-coordinated with a N<sub>4</sub>O<sub>2</sub> ligand set. The Etobb (1,3-bis(1-ethylbenzimidazol-2-yl)-2-oxopropane) ligand acts as a tridentate donor. The four N atoms are not in an ideal equatorial plane and the coordination geometry of the Co<sup>II</sup> may be best described as distorted octahedral. There are significant differences between chemically equivalent coordination bond lengths. The crystal structure is stabilized by weak intermolecular C—H...O hydrogen bond interactions and weak  $\pi\cdots\pi$  stacking interactions (Fig. 2) with centroid to centroid distances of 3.495 (1) Å between inversion related benzimidazole rings systems.

### Experimental

To a stirred solution of 1,3-bis(1-ethylbenzimidazol-2-yl)-2-oxopropane (0.167 g, 0.5 mmol) in hot MeOH (15 ml) was added Co(C<sub>6</sub>H<sub>2</sub>N<sub>3</sub>O<sub>7</sub>)<sub>2</sub> (0.129 g, 0.25 mmol) in MeOH (5 ml). A brown 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 DMF resulting in a brown solution. Brown crystals suitable for X-ray diffraction studies were obtained after three days at room temperature from ether diffusion into a DMF solution of the title compound. Yield, 0.210 g (71%). (found: C, 52.41; H, 4.68; N, 16.81. Calcd. for C<sub>116</sub>H<sub>124</sub>Co<sub>2</sub>N<sub>32</sub>O<sub>36</sub>: C, 52.37; H, 4.70; N, 16.85)

### 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 0.99 Å and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}$  or  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}$  of the carrier atom, respectively. In one of the anions one nitro group is rotationally disordered about the C-N bond with refined occupancies of 0.524 (8) [O8,O9] and 0.476 (8) [O8',O9'].

### Figures

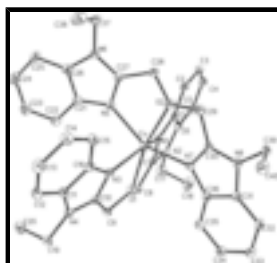


Fig. 1. Molecular structure and atom numbering for the cation of the title compound. Hydrogen atoms have been omitted for clarity and the displacement ellipsoids are shown at the 30% probability level.

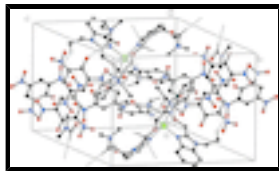


Fig. 2. Part of the crystal structure showing weak C—H...O hydrogen bonds (dashed lines) and weak  $\pi\cdots\pi$  stacking interactions. Only H atoms involved in hydrogen bonds are shown. The disorder is not shown.

## Bis[bis(1-ethylbenzimidazol-2-ylmethyl) ether]cobalt(II) dipicrate dimethylformamide disolvate

### Crystal data

|  |   |
|--|---|
| $[\text{Co}(\text{C}_{20}\text{H}_{22}\text{N}_4\text{O})_2](\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2 \cdot 2\text{C}_3\text{H}_7\text{NO}$ | $Z = 2$   |
| $M_r = 1330.17$  | $F_{000} = 1386$  |
| Triclinic, $P\bar{1}$  | $D_x = 1.446 \text{ Mg m}^{-3}$                         |
| Hall symbol: $-P\ 1$   | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 13.8799 (4) \text{ \AA}$  | Cell parameters from 7749 reflections                   |
| $b = 14.6525 (4) \text{ \AA}$  | $\theta = 3.0\text{--}25.5^\circ$                       |
| $c = 16.5701 (3) \text{ \AA}$  | $\mu = 0.37 \text{ mm}^{-1}$                            |
| $\alpha = 110.6640 (10)^\circ$   | $T = 153 \text{ K}$                                     |
| $\beta = 96.4700 (10)^\circ$   | Block, brown  |
| $\gamma = 99.6120 (10)^\circ$  | $0.38 \times 0.22 \times 0.14 \text{ mm}$               |
| $V = 3054.62 (13) \text{ \AA}^3$   |   |

### Data collection

|   |  |
|---|--|
| Rigaku R-Axis Spider diffractometer                       | 11225 independent reflections          |
| Radiation source: fine-focus sealed tube                  | 8833 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite                                   | $R_{\text{int}} = 0.022$               |
| $T = 153 \text{ K}$                                       | $\theta_{\text{max}} = 25.5^\circ$     |
| $\varphi$ and $\omega$ scans                              | $\theta_{\text{min}} = 3.0^\circ$      |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $h = -16 \rightarrow 16$               |
| $T_{\text{min}} = 0.873$ , $T_{\text{max}} = 0.950$       | $k = -17 \rightarrow 17$               |
| 24337 measured reflections                                | $l = -18 \rightarrow 20$               |

### Refinement

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | Secondary atom site location: difference Fourier map     |
| Least-squares matrix: full      | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | H-atom parameters constrained                            |
| $wR(F^2) = 0.136$               | $w = 1/[\sigma^2(F_o^2) + (0.0663P)^2 + 2.0559P]$        |
| $S = 1.14$                      | where $P = (F_o^2 + 2F_c^2)/3$                           |
| 11225 reflections               | $(\Delta/\sigma)_{\text{max}} = 0.10$                    |
| 858 parameters                  | $\Delta\rho_{\text{max}} = 0.98 \text{ e \AA}^{-3}$      |
|                                 | $\Delta\rho_{\text{min}} = -0.89 \text{ e \AA}^{-3}$     |

4 restraints

Extinction correction: SHELXL,  
 $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0022 (5)

*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.

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

|     | <i>x</i>     | <i>y</i>     | <i>z</i>      | $U_{iso}^*/U_{eq}$ | Occ. (<1) |
|-----|--------------|--------------|---------------|--------------------|-----------|
| Co  | 0.28649 (2)  | 0.19838 (2)  | 0.46816 (2)   | 0.01823 (11)       |           |
| O1  | 0.29902 (13) | 0.30499 (13) | 0.61018 (11)  | 0.0234 (4)         |           |
| O2  | 0.29752 (13) | 0.08087 (14) | 0.34517 (11)  | 0.0278 (4)         |           |
| O3  | 0.80117 (19) | 0.5715 (2)   | 0.13764 (15)  | 0.0629 (7)         |           |
| O4  | 0.5964 (3)   | 0.3781 (2)   | 0.17574 (16)  | 0.0752 (10)        |           |
| O5  | 0.7548 (3)   | 0.4037 (3)   | 0.1790 (2)    | 0.0980 (12)        |           |
| O6  | 0.41385 (18) | 0.2944 (2)   | -0.11930 (18) | 0.0619 (7)         |           |
| O7  | 0.45343 (19) | 0.3970 (2)   | -0.18404 (14) | 0.0559 (7)         |           |
| O8  | 0.7909 (5)   | 0.6140 (5)   | -0.0805 (3)   | 0.082 (3)          | 0.524 (8) |
| O9  | 0.8201 (4)   | 0.6944 (5)   | 0.0537 (4)    | 0.064 (2)          | 0.524 (8) |
| O8' | 0.7091 (5)   | 0.6837 (5)   | -0.0389 (4)   | 0.089 (3)          | 0.476 (8) |
| O9' | 0.8490 (4)   | 0.6593 (10)  | 0.0175 (9)    | 0.116 (4)          | 0.476 (8) |
| O10 | 0.67849 (16) | 0.05378 (17) | -0.11405 (13) | 0.0406 (5)         |           |
| O11 | 0.54090 (17) | 0.13588 (18) | -0.18370 (13) | 0.0434 (5)         |           |
| O12 | 0.40246 (16) | 0.06268 (18) | -0.16289 (14) | 0.0443 (5)         |           |
| O13 | 0.39642 (17) | 0.17501 (17) | 0.15142 (14)  | 0.0442 (5)         |           |
| O14 | 0.52461 (17) | 0.17492 (16) | 0.23989 (12)  | 0.0407 (5)         |           |
| O15 | 0.80210 (18) | 0.0547 (2)   | 0.11187 (18)  | 0.0587 (7)         |           |
| O16 | 0.84422 (16) | 0.1175 (2)   | 0.01821 (15)  | 0.0518 (6)         |           |
| O17 | 0.10881 (18) | 0.8163 (2)   | 0.20909 (15)  | 0.0575 (7)         |           |
| O18 | 0.07622 (17) | 0.40600 (18) | 0.63580 (14)  | 0.0473 (6)         |           |
| N1  | 0.20049 (14) | 0.12155 (16) | 0.52909 (12)  | 0.0197 (4)         |           |
| N2  | 0.14353 (15) | 0.10419 (16) | 0.64503 (13)  | 0.0223 (5)         |           |
| N3  | 0.33896 (15) | 0.34492 (15) | 0.47641 (13)  | 0.0200 (4)         |           |
| N4  | 0.36761 (15) | 0.51053 (15) | 0.54120 (13)  | 0.0209 (4)         |           |
| N5  | 0.16690 (15) | 0.19040 (16) | 0.36748 (13)  | 0.0206 (4)         |           |
| N6  | 0.09391 (16) | 0.13339 (17) | 0.22634 (13)  | 0.0248 (5)         |           |
| N7  | 0.42207 (15) | 0.15693 (15) | 0.49147 (12)  | 0.0196 (4)         |           |
| N8  | 0.54212 (16) | 0.07996 (16) | 0.44281 (13)  | 0.0235 (5)         |           |

## supplementary materials

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|      |              |              |               |             |
|------|--------------|--------------|---------------|-------------|
| N9   | 0.6710 (3)   | 0.4043 (2)   | 0.14874 (18)  | 0.0558 (9)  |
| N10  | 0.4692 (2)   | 0.3651 (2)   | -0.12503 (18) | 0.0426 (7)  |
| N11  | 0.7593 (3)   | 0.6329 (3)   | -0.01009 (19) | 0.0867 (15) |
| N12  | 0.49148 (18) | 0.10217 (18) | -0.13969 (14) | 0.0321 (5)  |
| N13  | 0.48254 (19) | 0.16547 (18) | 0.16615 (15)  | 0.0327 (6)  |
| N14  | 0.78255 (18) | 0.0908 (2)   | 0.05747 (16)  | 0.0370 (6)  |
| N15  | 0.1137 (2)   | 0.7045 (3)   | 0.07460 (19)  | 0.0623 (9)  |
| N16  | -0.0601 (2)  | 0.4302 (2)   | 0.69697 (17)  | 0.0453 (7)  |
| C1   | 0.14755 (17) | 0.02311 (19) | 0.50421 (16)  | 0.0202 (5)  |
| C2   | 0.12581 (18) | -0.0567 (2)  | 0.42273 (16)  | 0.0237 (5)  |
| H2A  | 0.1477       | -0.0491      | 0.3727        | 0.028*      |
| C3   | 0.07159 (19) | -0.1465 (2)  | 0.41792 (18)  | 0.0278 (6)  |
| H3A  | 0.0565       | -0.2020      | 0.3635        | 0.033*      |
| C4   | 0.0378 (2)   | -0.1586 (2)  | 0.49117 (18)  | 0.0289 (6)  |
| H4A  | 0.0010       | -0.2222      | 0.4853        | 0.035*      |
| C5   | 0.05712 (19) | -0.0795 (2)  | 0.57183 (18)  | 0.0282 (6)  |
| H5A  | 0.0339       | -0.0869      | 0.6214        | 0.034*      |
| C6   | 0.11200 (18) | 0.01088 (19) | 0.57638 (16)  | 0.0220 (5)  |
| C7   | 0.19536 (17) | 0.16562 (19) | 0.61295 (15)  | 0.0194 (5)  |
| C8   | 0.24117 (19) | 0.27325 (19) | 0.66549 (15)  | 0.0224 (5)  |
| H8A  | 0.1893       | 0.3122       | 0.6799        | 0.027*      |
| H8B  | 0.2838       | 0.2815       | 0.7208        | 0.027*      |
| C9   | 0.3238 (2)   | 0.40958 (18) | 0.63268 (15)  | 0.0229 (5)  |
| H9A  | 0.3830       | 0.4412       | 0.6802        | 0.028*      |
| H9B  | 0.2677       | 0.4400       | 0.6523        | 0.028*      |
| C10  | 0.34504 (17) | 0.42222 (19) | 0.55015 (15)  | 0.0206 (5)  |
| C11  | 0.37509 (18) | 0.48952 (19) | 0.45373 (16)  | 0.0223 (5)  |
| C12  | 0.3948 (2)   | 0.5512 (2)   | 0.40767 (18)  | 0.0291 (6)  |
| H12A | 0.4070       | 0.6220       | 0.4351        | 0.035*      |
| C13  | 0.3958 (2)   | 0.5032 (2)   | 0.31901 (18)  | 0.0346 (7)  |
| H13A | 0.4087       | 0.5425       | 0.2848        | 0.041*      |
| C14  | 0.3782 (2)   | 0.3990 (2)   | 0.27845 (18)  | 0.0315 (6)  |
| H14A | 0.3796       | 0.3693       | 0.2177        | 0.038*      |
| C15  | 0.3590 (2)   | 0.3387 (2)   | 0.32506 (17)  | 0.0271 (6)  |
| H15A | 0.3475       | 0.2679       | 0.2977        | 0.033*      |
| C16  | 0.35722 (18) | 0.38544 (19) | 0.41382 (16)  | 0.0221 (5)  |
| C17  | 0.1169 (2)   | 0.1340 (2)   | 0.73351 (17)  | 0.0282 (6)  |
| H17A | 0.0446       | 0.1088       | 0.7274        | 0.034*      |
| H17B | 0.1312       | 0.2079       | 0.7612        | 0.034*      |
| C18  | 0.1725 (3)   | 0.0947 (3)   | 0.7923 (2)    | 0.0495 (9)  |
| H18A | 0.1522       | 0.1163       | 0.8497        | 0.074*      |
| H18B | 0.2441       | 0.1207       | 0.7998        | 0.074*      |
| H18C | 0.1576       | 0.0215       | 0.7659        | 0.074*      |
| C19  | 0.3731 (2)   | 0.60909 (19) | 0.60915 (16)  | 0.0263 (6)  |
| H19A | 0.4201       | 0.6604       | 0.5984        | 0.032*      |
| H19B | 0.3991       | 0.6091       | 0.6673        | 0.032*      |
| C20  | 0.2727 (2)   | 0.6357 (2)   | 0.6101 (2)    | 0.0423 (8)  |
| H20A | 0.2791       | 0.7016       | 0.6563        | 0.063*      |
| H20B | 0.2262       | 0.5855       | 0.6215        | 0.063*      |

|      |              |              |               |            |
|------|--------------|--------------|---------------|------------|
| H20C | 0.2475       | 0.6374       | 0.5531        | 0.063*     |
| C21  | 0.09872 (18) | 0.24717 (19) | 0.35843 (15)  | 0.0217 (5) |
| C22  | 0.0729 (2)   | 0.3280 (2)   | 0.42065 (17)  | 0.0274 (6) |
| H22A | 0.1039       | 0.3535       | 0.4807        | 0.033*     |
| C23  | 0.0009 (2)   | 0.3692 (2)   | 0.39152 (19)  | 0.0341 (7) |
| H23A | -0.0183      | 0.4237       | 0.4326        | 0.041*     |
| C24  | -0.0450 (2)  | 0.3330 (2)   | 0.30304 (19)  | 0.0363 (7) |
| H24A | -0.0944      | 0.3636       | 0.2857        | 0.044*     |
| C25  | -0.0199 (2)  | 0.2536 (2)   | 0.24042 (19)  | 0.0332 (6) |
| H25A | -0.0503      | 0.2289       | 0.1802        | 0.040*     |
| C26  | 0.05232 (19) | 0.2121 (2)   | 0.27061 (16)  | 0.0251 (6) |
| C27  | 0.16210 (18) | 0.12508 (19) | 0.28700 (15)  | 0.0221 (5) |
| C28  | 0.22980 (19) | 0.0551 (2)   | 0.26444 (16)  | 0.0259 (6) |
| H28A | 0.1923       | -0.0153      | 0.2432        | 0.031*     |
| H28B | 0.2658       | 0.0642       | 0.2186        | 0.031*     |
| C29  | 0.38727 (18) | 0.0477 (2)   | 0.33422 (16)  | 0.0233 (5) |
| H29A | 0.4191       | 0.0695       | 0.2916        | 0.028*     |
| H29B | 0.3748       | -0.0261      | 0.3134        | 0.028*     |
| C30  | 0.45091 (18) | 0.09541 (18) | 0.42356 (15)  | 0.0195 (5) |
| C31  | 0.57725 (19) | 0.13738 (19) | 0.53148 (16)  | 0.0233 (5) |
| C32  | 0.6663 (2)   | 0.1502 (2)   | 0.58537 (18)  | 0.0298 (6) |
| H32A | 0.7174       | 0.1183       | 0.5633        | 0.036*     |
| C33  | 0.6775 (2)   | 0.2111 (2)   | 0.67244 (18)  | 0.0306 (6) |
| H33A | 0.7376       | 0.2219       | 0.7115        | 0.037*     |
| C34  | 0.6014 (2)   | 0.2577 (2)   | 0.70433 (17)  | 0.0286 (6) |
| H34A | 0.6113       | 0.2992       | 0.7647        | 0.034*     |
| C35  | 0.51260 (19) | 0.2449 (2)   | 0.65041 (16)  | 0.0251 (6) |
| H35A | 0.4612       | 0.2760       | 0.6727        | 0.030*     |
| C36  | 0.50137 (18) | 0.18448 (19) | 0.56205 (15)  | 0.0204 (5) |
| C37  | 0.0750 (2)   | 0.0776 (2)   | 0.13075 (16)  | 0.0333 (7) |
| H37A | 0.0028       | 0.0625       | 0.1076        | 0.040*     |
| H37B | 0.0957       | 0.0133       | 0.1182        | 0.040*     |
| C38  | 0.1305 (3)   | 0.1359 (3)   | 0.0843 (2)    | 0.0502 (9) |
| H38A | 0.1163       | 0.0963       | 0.0211        | 0.075*     |
| H38B | 0.2021       | 0.1501       | 0.1065        | 0.075*     |
| H38C | 0.1090       | 0.1989       | 0.0954        | 0.075*     |
| C39  | 0.6008 (2)   | 0.0221 (2)   | 0.38379 (17)  | 0.0279 (6) |
| H39A | 0.5560       | -0.0255      | 0.3289        | 0.033*     |
| H39B | 0.6329       | -0.0173      | 0.4121        | 0.033*     |
| C40  | 0.6796 (2)   | 0.0891 (2)   | 0.36196 (19)  | 0.0363 (7) |
| H40A | 0.7171       | 0.0482       | 0.3226        | 0.055*     |
| H40B | 0.7249       | 0.1353       | 0.4161        | 0.055*     |
| H40C | 0.6479       | 0.1273       | 0.3330        | 0.055*     |
| C41  | 0.7297 (2)   | 0.5228 (2)   | 0.07784 (18)  | 0.0378 (7) |
| C42  | 0.6578 (2)   | 0.4375 (2)   | 0.07595 (17)  | 0.0350 (7) |
| C43  | 0.5747 (2)   | 0.3879 (2)   | 0.01257 (18)  | 0.0330 (6) |
| H43A | 0.5291       | 0.3348       | 0.0173        | 0.040*     |
| C44  | 0.5576 (2)   | 0.4155 (2)   | -0.05849 (17) | 0.0310 (6) |
| C45  | 0.6213 (2)   | 0.4953 (2)   | -0.06346 (17) | 0.0367 (7) |

## supplementary materials

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|      |             |            |               |             |
|------|-------------|------------|---------------|-------------|
| H45A | 0.6087      | 0.5148     | -0.1118       | 0.044*      |
| C46  | 0.7027 (2)  | 0.5462 (2) | 0.00134 (19)  | 0.0388 (7)  |
| C47  | 0.6395 (2)  | 0.0877 (2) | -0.04959 (17) | 0.0278 (6)  |
| C48  | 0.5411 (2)  | 0.1095 (2) | -0.05470 (16) | 0.0265 (6)  |
| C49  | 0.4898 (2)  | 0.1320 (2) | 0.01257 (16)  | 0.0264 (6)  |
| H49A | 0.4240      | 0.1413     | 0.0034        | 0.032*      |
| C50  | 0.5358 (2)  | 0.1411 (2) | 0.09506 (16)  | 0.0261 (6)  |
| C51  | 0.6320 (2)  | 0.1276 (2) | 0.10885 (17)  | 0.0293 (6)  |
| H51A | 0.6629      | 0.1342     | 0.1654        | 0.035*      |
| C52  | 0.6820 (2)  | 0.1045 (2) | 0.04027 (17)  | 0.0286 (6)  |
| C53  | 0.0698 (3)  | 0.7568 (4) | 0.1365 (3)    | 0.0910 (19) |
| H53  | -0.0004     | 0.7463     | 0.1222        | 0.109*      |
| C54  | 0.2175 (3)  | 0.7168 (3) | 0.0886 (2)    | 0.0534 (9)  |
| H54A | 0.2460      | 0.7619     | 0.1493        | 0.080*      |
| H54B | 0.2447      | 0.7454     | 0.0484        | 0.080*      |
| H54C | 0.2344      | 0.6517     | 0.0777        | 0.080*      |
| C55  | 0.0620 (4)  | 0.6385 (6) | -0.0135 (4)   | 0.162 (4)   |
| H55A | -0.0096     | 0.6347     | -0.0175       | 0.242*      |
| H55B | 0.0749      | 0.5715     | -0.0262       | 0.242*      |
| H55C | 0.0860      | 0.6648     | -0.0561       | 0.242*      |
| C56  | 0.0356 (2)  | 0.4296 (2) | 0.6990 (2)    | 0.0416 (8)  |
| H56A | 0.0762      | 0.4495     | 0.7551        | 0.050*      |
| C57  | -0.1274 (3) | 0.4030 (3) | 0.6141 (2)    | 0.0497 (8)  |
| H57A | -0.0914     | 0.3820     | 0.5656        | 0.075*      |
| H57B | -0.1538     | 0.4608     | 0.6136        | 0.075*      |
| H57C | -0.1825     | 0.3478     | 0.6074        | 0.075*      |
| C58  | -0.1011 (4) | 0.4648 (4) | 0.7763 (3)    | 0.099 (2)   |
| H58A | -0.0493     | 0.4805     | 0.8275        | 0.149*      |
| H58B | -0.1562     | 0.4123     | 0.7746        | 0.149*      |
| H58C | -0.1255     | 0.5250     | 0.7803        | 0.149*      |

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

|     | $U^{11}$     | $U^{22}$    | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|--------------|-------------|--------------|--------------|--------------|--------------|
| Co  | 0.01811 (18) | 0.0209 (2)  | 0.01589 (17) | 0.00583 (13) | 0.00398 (12) | 0.00627 (13) |
| O1  | 0.0314 (10)  | 0.0197 (9)  | 0.0205 (9)   | 0.0050 (8)   | 0.0116 (7)   | 0.0075 (7)   |
| O2  | 0.0226 (10)  | 0.0405 (12) | 0.0179 (9)   | 0.0166 (8)   | 0.0030 (7)   | 0.0040 (8)   |
| O3  | 0.0526 (16)  | 0.0693 (18) | 0.0400 (13)  | -0.0042 (13) | -0.0136 (11) | 0.0035 (12)  |
| O4  | 0.139 (3)    | 0.0478 (16) | 0.0359 (14)  | 0.0037 (17)  | 0.0277 (16)  | 0.0170 (12)  |
| O5  | 0.126 (3)    | 0.106 (3)   | 0.068 (2)    | 0.041 (2)    | -0.024 (2)   | 0.0462 (19)  |
| O6  | 0.0374 (14)  | 0.0474 (16) | 0.0740 (18)  | 0.0025 (12)  | -0.0019 (12) | -0.0022 (13) |
| O7  | 0.0561 (16)  | 0.0713 (18) | 0.0288 (12)  | 0.0351 (14)  | -0.0065 (10) | 0.0000 (11)  |
| O8  | 0.089 (5)    | 0.081 (5)   | 0.070 (4)    | -0.009 (4)   | 0.038 (3)    | 0.028 (3)    |
| O9  | 0.033 (3)    | 0.051 (4)   | 0.093 (5)    | -0.008 (3)   | 0.000 (3)    | 0.020 (3)    |
| O8' | 0.115 (6)    | 0.078 (5)   | 0.076 (5)    | -0.031 (4)   | -0.014 (4)   | 0.065 (4)    |
| O9' | 0.072 (6)    | 0.120 (10)  | 0.160 (11)   | -0.004 (6)   | 0.033 (6)    | 0.066 (8)    |
| O10 | 0.0462 (13)  | 0.0484 (14) | 0.0297 (11)  | 0.0229 (11)  | 0.0162 (9)   | 0.0094 (9)   |
| O11 | 0.0488 (13)  | 0.0599 (15) | 0.0291 (11)  | 0.0127 (11)  | 0.0105 (9)   | 0.0248 (10)  |

|     |             |             |             |             |              |              |
|-----|-------------|-------------|-------------|-------------|--------------|--------------|
| O12 | 0.0330 (13) | 0.0553 (15) | 0.0398 (12) | 0.0022 (11) | -0.0048 (9)  | 0.0194 (10)  |
| O13 | 0.0399 (13) | 0.0526 (15) | 0.0425 (12) | 0.0184 (11) | 0.0209 (10)  | 0.0132 (10)  |
| O14 | 0.0554 (14) | 0.0444 (13) | 0.0219 (10) | 0.0091 (11) | 0.0129 (9)   | 0.0113 (9)   |
| O15 | 0.0397 (14) | 0.085 (2)   | 0.0775 (18) | 0.0222 (13) | 0.0072 (12)  | 0.0592 (16)  |
| O16 | 0.0307 (12) | 0.0788 (19) | 0.0536 (14) | 0.0140 (12) | 0.0156 (10)  | 0.0312 (13)  |
| O17 | 0.0457 (14) | 0.0662 (17) | 0.0402 (13) | 0.0142 (13) | 0.0072 (11)  | -0.0046 (12) |
| O18 | 0.0415 (13) | 0.0523 (15) | 0.0379 (12) | 0.0189 (11) | 0.0043 (10)  | 0.0022 (10)  |
| N1  | 0.0158 (10) | 0.0250 (12) | 0.0176 (10) | 0.0064 (9)  | 0.0028 (8)   | 0.0065 (8)   |
| N2  | 0.0191 (11) | 0.0300 (12) | 0.0197 (10) | 0.0054 (9)  | 0.0062 (8)   | 0.0110 (9)   |
| N3  | 0.0202 (11) | 0.0198 (11) | 0.0194 (10) | 0.0015 (9)  | 0.0039 (8)   | 0.0079 (8)   |
| N4  | 0.0234 (11) | 0.0159 (11) | 0.0222 (11) | 0.0032 (9)  | 0.0038 (8)   | 0.0063 (8)   |
| N5  | 0.0191 (11) | 0.0229 (11) | 0.0190 (10) | 0.0051 (9)  | 0.0044 (8)   | 0.0065 (8)   |
| N6  | 0.0232 (11) | 0.0322 (13) | 0.0166 (10) | 0.0101 (10) | 0.0012 (8)   | 0.0056 (9)   |
| N7  | 0.0190 (11) | 0.0223 (11) | 0.0180 (10) | 0.0060 (9)  | 0.0046 (8)   | 0.0072 (8)   |
| N8  | 0.0220 (11) | 0.0263 (12) | 0.0229 (11) | 0.0103 (9)  | 0.0046 (8)   | 0.0078 (9)   |
| N9  | 0.099 (3)   | 0.0392 (17) | 0.0260 (14) | 0.0201 (17) | 0.0034 (16)  | 0.0089 (12)  |
| N10 | 0.0321 (15) | 0.0375 (16) | 0.0414 (16) | 0.0165 (13) | 0.0017 (11)  | -0.0074 (12) |
| N11 | 0.117 (4)   | 0.079 (3)   | 0.0377 (19) | -0.042 (3)  | 0.007 (2)    | 0.0219 (18)  |
| N12 | 0.0365 (14) | 0.0349 (14) | 0.0244 (12) | 0.0123 (11) | 0.0051 (10)  | 0.0090 (10)  |
| N13 | 0.0414 (15) | 0.0270 (13) | 0.0284 (13) | 0.0057 (11) | 0.0148 (11)  | 0.0073 (10)  |
| N14 | 0.0309 (14) | 0.0438 (16) | 0.0405 (14) | 0.0118 (12) | 0.0058 (11)  | 0.0196 (12)  |
| N15 | 0.0422 (17) | 0.064 (2)   | 0.0459 (17) | 0.0149 (15) | -0.0057 (13) | -0.0179 (15) |
| N16 | 0.0410 (16) | 0.0472 (17) | 0.0354 (14) | 0.0045 (13) | 0.0070 (11)  | 0.0037 (12)  |
| C1  | 0.0131 (12) | 0.0231 (13) | 0.0263 (13) | 0.0063 (10) | 0.0029 (9)   | 0.0110 (10)  |
| C2  | 0.0159 (12) | 0.0313 (15) | 0.0234 (13) | 0.0079 (11) | 0.0034 (9)   | 0.0087 (11)  |
| C3  | 0.0222 (14) | 0.0249 (14) | 0.0318 (14) | 0.0080 (11) | -0.0003 (10) | 0.0058 (11)  |
| C4  | 0.0234 (14) | 0.0220 (14) | 0.0408 (16) | 0.0025 (11) | 0.0024 (11)  | 0.0138 (12)  |
| C5  | 0.0218 (14) | 0.0323 (16) | 0.0366 (15) | 0.0064 (12) | 0.0060 (11)  | 0.0201 (12)  |
| C6  | 0.0149 (12) | 0.0261 (14) | 0.0252 (13) | 0.0055 (10) | 0.0025 (9)   | 0.0101 (10)  |
| C7  | 0.0170 (12) | 0.0238 (13) | 0.0188 (12) | 0.0070 (10) | 0.0038 (9)   | 0.0087 (10)  |
| C8  | 0.0245 (13) | 0.0247 (14) | 0.0165 (12) | 0.0032 (11) | 0.0068 (9)   | 0.0062 (10)  |
| C9  | 0.0290 (14) | 0.0168 (13) | 0.0199 (12) | 0.0037 (11) | 0.0040 (10)  | 0.0039 (10)  |
| C10 | 0.0159 (12) | 0.0248 (14) | 0.0191 (12) | 0.0043 (10) | 0.0015 (9)   | 0.0064 (10)  |
| C11 | 0.0185 (13) | 0.0221 (13) | 0.0259 (13) | 0.0027 (10) | 0.0049 (10)  | 0.0091 (10)  |
| C12 | 0.0330 (15) | 0.0230 (14) | 0.0337 (15) | 0.0056 (12) | 0.0082 (11)  | 0.0133 (11)  |
| C13 | 0.0389 (17) | 0.0405 (18) | 0.0329 (15) | 0.0069 (14) | 0.0124 (12)  | 0.0232 (13)  |
| C14 | 0.0387 (16) | 0.0347 (16) | 0.0241 (13) | 0.0079 (13) | 0.0123 (11)  | 0.0129 (12)  |
| C15 | 0.0302 (15) | 0.0257 (14) | 0.0254 (13) | 0.0073 (12) | 0.0091 (11)  | 0.0078 (11)  |
| C16 | 0.0176 (12) | 0.0256 (14) | 0.0242 (13) | 0.0049 (10) | 0.0051 (9)   | 0.0105 (10)  |
| C17 | 0.0264 (14) | 0.0394 (17) | 0.0244 (13) | 0.0104 (12) | 0.0111 (11)  | 0.0155 (12)  |
| C18 | 0.059 (2)   | 0.073 (3)   | 0.0339 (17) | 0.0341 (19) | 0.0170 (15)  | 0.0302 (17)  |
| C19 | 0.0324 (15) | 0.0192 (14) | 0.0239 (13) | 0.0041 (11) | 0.0059 (11)  | 0.0048 (10)  |
| C20 | 0.0413 (18) | 0.0342 (18) | 0.0475 (18) | 0.0171 (15) | 0.0096 (14)  | 0.0067 (14)  |
| C21 | 0.0180 (12) | 0.0268 (14) | 0.0215 (12) | 0.0044 (11) | 0.0053 (9)   | 0.0104 (10)  |
| C22 | 0.0272 (14) | 0.0306 (15) | 0.0255 (13) | 0.0092 (12) | 0.0083 (10)  | 0.0096 (11)  |
| C23 | 0.0337 (16) | 0.0365 (17) | 0.0357 (16) | 0.0163 (13) | 0.0127 (12)  | 0.0124 (13)  |
| C24 | 0.0321 (16) | 0.0439 (19) | 0.0404 (16) | 0.0198 (14) | 0.0075 (12)  | 0.0196 (14)  |
| C25 | 0.0275 (15) | 0.0430 (18) | 0.0307 (15) | 0.0145 (13) | 0.0017 (11)  | 0.0140 (13)  |
| C26 | 0.0232 (14) | 0.0293 (15) | 0.0224 (13) | 0.0070 (11) | 0.0046 (10)  | 0.0085 (11)  |

## supplementary materials

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|     |             |             |             |              |              |              |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C27 | 0.0183 (12) | 0.0264 (14) | 0.0183 (12) | 0.0038 (10)  | 0.0024 (9)   | 0.0055 (10)  |
| C28 | 0.0236 (14) | 0.0328 (15) | 0.0163 (12) | 0.0096 (11)  | -0.0005 (10) | 0.0033 (10)  |
| C29 | 0.0220 (13) | 0.0281 (14) | 0.0211 (12) | 0.0108 (11)  | 0.0077 (10)  | 0.0076 (10)  |
| C30 | 0.0198 (13) | 0.0173 (13) | 0.0239 (12) | 0.0048 (10)  | 0.0066 (10)  | 0.0099 (10)  |
| C31 | 0.0223 (13) | 0.0234 (14) | 0.0242 (13) | 0.0047 (11)  | 0.0032 (10)  | 0.0095 (10)  |
| C32 | 0.0245 (14) | 0.0348 (16) | 0.0336 (15) | 0.0129 (12)  | 0.0049 (11)  | 0.0145 (12)  |
| C33 | 0.0266 (15) | 0.0321 (16) | 0.0307 (14) | 0.0058 (12)  | -0.0032 (11) | 0.0117 (12)  |
| C34 | 0.0317 (15) | 0.0285 (15) | 0.0234 (13) | 0.0062 (12)  | 0.0012 (11)  | 0.0085 (11)  |
| C35 | 0.0249 (14) | 0.0286 (15) | 0.0239 (13) | 0.0071 (11)  | 0.0067 (10)  | 0.0113 (11)  |
| C36 | 0.0202 (13) | 0.0205 (13) | 0.0215 (12) | 0.0032 (10)  | 0.0031 (9)   | 0.0100 (10)  |
| C37 | 0.0302 (15) | 0.0452 (18) | 0.0164 (13) | 0.0120 (13)  | -0.0031 (10) | 0.0028 (12)  |
| C38 | 0.053 (2)   | 0.070 (3)   | 0.0279 (16) | 0.0150 (18)  | 0.0104 (14)  | 0.0173 (16)  |
| C39 | 0.0272 (14) | 0.0299 (15) | 0.0280 (14) | 0.0170 (12)  | 0.0071 (11)  | 0.0072 (11)  |
| C40 | 0.0296 (16) | 0.0451 (19) | 0.0368 (16) | 0.0135 (14)  | 0.0137 (12)  | 0.0138 (13)  |
| C41 | 0.0352 (17) | 0.0419 (18) | 0.0256 (14) | 0.0057 (14)  | 0.0027 (12)  | 0.0023 (12)  |
| C42 | 0.0490 (19) | 0.0379 (17) | 0.0203 (13) | 0.0196 (14)  | 0.0074 (12)  | 0.0088 (12)  |
| C43 | 0.0399 (17) | 0.0237 (15) | 0.0342 (15) | 0.0115 (13)  | 0.0138 (12)  | 0.0055 (12)  |
| C44 | 0.0299 (15) | 0.0321 (16) | 0.0232 (13) | 0.0129 (13)  | 0.0006 (11)  | -0.0004 (11) |
| C45 | 0.0517 (19) | 0.0356 (17) | 0.0189 (13) | 0.0081 (14)  | 0.0042 (12)  | 0.0072 (12)  |
| C46 | 0.0436 (18) | 0.0348 (17) | 0.0306 (15) | -0.0025 (14) | 0.0094 (13)  | 0.0080 (13)  |
| C47 | 0.0317 (15) | 0.0265 (15) | 0.0263 (14) | 0.0110 (12)  | 0.0095 (11)  | 0.0081 (11)  |
| C48 | 0.0317 (15) | 0.0258 (14) | 0.0204 (13) | 0.0075 (12)  | 0.0028 (10)  | 0.0071 (10)  |
| C49 | 0.0273 (14) | 0.0262 (14) | 0.0262 (13) | 0.0082 (11)  | 0.0066 (11)  | 0.0092 (11)  |
| C50 | 0.0329 (15) | 0.0262 (14) | 0.0214 (13) | 0.0085 (12)  | 0.0095 (11)  | 0.0094 (10)  |
| C51 | 0.0329 (15) | 0.0313 (16) | 0.0229 (13) | 0.0052 (12)  | 0.0039 (11)  | 0.0105 (11)  |
| C52 | 0.0257 (14) | 0.0303 (15) | 0.0301 (14) | 0.0084 (12)  | 0.0052 (11)  | 0.0108 (11)  |
| C53 | 0.040 (2)   | 0.113 (4)   | 0.067 (3)   | 0.030 (2)    | -0.0079 (19) | -0.030 (3)   |
| C54 | 0.053 (2)   | 0.057 (2)   | 0.0446 (19) | 0.0150 (18)  | 0.0175 (16)  | 0.0084 (16)  |
| C55 | 0.083 (4)   | 0.187 (7)   | 0.093 (4)   | 0.039 (4)    | -0.027 (3)   | -0.082 (4)   |
| C56 | 0.046 (2)   | 0.0370 (18) | 0.0321 (16) | 0.0078 (15)  | -0.0047 (14) | 0.0058 (13)  |
| C57 | 0.0376 (19) | 0.052 (2)   | 0.059 (2)   | 0.0071 (16)  | -0.0016 (15) | 0.0237 (17)  |
| C58 | 0.071 (3)   | 0.108 (4)   | 0.066 (3)   | -0.019 (3)   | 0.036 (2)    | -0.018 (3)   |

### *Geometric parameters (Å, °)*

|        |             |          |           |
|--------|-------------|----------|-----------|
| Co—N1  | 2.083 (2)   | C13—H13A | 0.9500    |
| Co—N3  | 2.099 (2)   | C14—C15  | 1.378 (4) |
| Co—N7  | 2.108 (2)   | C14—H14A | 0.9500    |
| Co—N5  | 2.174 (2)   | C15—C16  | 1.391 (4) |
| Co—O2  | 2.1961 (17) | C15—H15A | 0.9500    |
| Co—O1  | 2.2872 (16) | C17—C18  | 1.501 (4) |
| O1—C9  | 1.413 (3)   | C17—H17A | 0.9900    |
| O1—C8  | 1.429 (3)   | C17—H17B | 0.9900    |
| O2—C29 | 1.419 (3)   | C18—H18A | 0.9800    |
| O2—C28 | 1.434 (3)   | C18—H18B | 0.9800    |
| O3—C41 | 1.232 (4)   | C18—H18C | 0.9800    |
| O4—N9  | 1.230 (4)   | C19—C20  | 1.510 (4) |
| O5—N9  | 1.217 (5)   | C19—H19A | 0.9900    |
| O6—N10 | 1.222 (4)   | C19—H19B | 0.9900    |

|         |           |          |           |
|---------|-----------|----------|-----------|
| O7—N10  | 1.237 (4) | C20—H20A | 0.9800    |
| O8—N11  | 1.249 (3) | C20—H20B | 0.9800    |
| O9—N11  | 1.230 (3) | C20—H20C | 0.9800    |
| O8'—N11 | 1.271 (3) | C21—C26  | 1.395 (3) |
| O9'—N11 | 1.223 (3) | C21—C22  | 1.399 (4) |
| O10—C47 | 1.236 (3) | C22—C23  | 1.376 (4) |
| O11—N12 | 1.225 (3) | C22—H22A | 0.9500    |
| O12—N12 | 1.227 (3) | C23—C24  | 1.402 (4) |
| O13—O13 | 0.000 (5) | C23—H23A | 0.9500    |
| O13—N13 | 1.234 (3) | C24—C25  | 1.384 (4) |
| O14—O14 | 0.000 (5) | C24—H24A | 0.9500    |
| O14—N13 | 1.243 (3) | C25—C26  | 1.389 (4) |
| O15—N14 | 1.223 (3) | C25—H25A | 0.9500    |
| O16—N14 | 1.226 (3) | C27—C28  | 1.485 (4) |
| O17—C53 | 1.206 (4) | C28—H28A | 0.9900    |
| O18—C56 | 1.216 (4) | C28—H28B | 0.9900    |
| N1—C7   | 1.326 (3) | C29—C30  | 1.493 (3) |
| N1—C1   | 1.396 (3) | C29—H29A | 0.9900    |
| N2—C7   | 1.348 (3) | C29—H29B | 0.9900    |
| N2—C6   | 1.395 (3) | C31—C32  | 1.384 (4) |
| N2—C17  | 1.484 (3) | C31—C36  | 1.399 (4) |
| N3—C10  | 1.323 (3) | C32—C33  | 1.378 (4) |
| N3—C16  | 1.391 (3) | C32—H32A | 0.9500    |
| N4—C10  | 1.343 (3) | C33—C34  | 1.404 (4) |
| N4—C11  | 1.391 (3) | C33—H33A | 0.9500    |
| N4—C19  | 1.468 (3) | C34—C35  | 1.382 (4) |
| N5—C27  | 1.325 (3) | C34—H34A | 0.9500    |
| N5—C21  | 1.389 (3) | C35—C36  | 1.392 (3) |
| N6—C27  | 1.353 (3) | C35—H35A | 0.9500    |
| N6—C26  | 1.387 (3) | C37—C38  | 1.513 (4) |
| N6—C37  | 1.472 (3) | C37—H37A | 0.9900    |
| N7—C30  | 1.321 (3) | C37—H37B | 0.9900    |
| N7—C36  | 1.404 (3) | C38—H38A | 0.9800    |
| N8—C30  | 1.346 (3) | C38—H38B | 0.9800    |
| N8—C31  | 1.391 (3) | C38—H38C | 0.9800    |
| N8—C39  | 1.472 (3) | C39—C40  | 1.507 (4) |
| N9—C42  | 1.455 (4) | C39—H39A | 0.9900    |
| N10—C44 | 1.444 (4) | C39—H39B | 0.9900    |
| N11—C46 | 1.463 (4) | C40—H40A | 0.9800    |
| N12—C48 | 1.456 (3) | C40—H40B | 0.9800    |
| N13—O13 | 1.234 (3) | C40—H40C | 0.9800    |
| N13—O14 | 1.243 (3) | C41—C46  | 1.452 (4) |
| N13—C50 | 1.432 (3) | C41—C42  | 1.452 (4) |
| N14—C52 | 1.454 (4) | C42—C43  | 1.367 (4) |
| N15—C53 | 1.324 (5) | C43—C44  | 1.383 (4) |
| N15—C54 | 1.405 (5) | C43—H43A | 0.9500    |
| N15—C55 | 1.455 (5) | C44—C45  | 1.375 (4) |
| N16—C56 | 1.327 (4) | C45—C46  | 1.366 (4) |
| N16—C58 | 1.450 (5) | C45—H45A | 0.9500    |

## supplementary materials

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|             |             |               |           |
|-------------|-------------|---------------|-----------|
| N16—C57     | 1.455 (4)   | C47—C48       | 1.453 (4) |
| C1—C2       | 1.400 (4)   | C47—C52       | 1.456 (4) |
| C1—C6       | 1.400 (3)   | C48—C49       | 1.362 (4) |
| C2—C3       | 1.372 (4)   | C49—C50       | 1.393 (4) |
| C2—H2A      | 0.9500      | C49—H49A      | 0.9500    |
| C3—C4       | 1.407 (4)   | C50—C51       | 1.388 (4) |
| C3—H3A      | 0.9500      | C51—C52       | 1.368 (4) |
| C4—C5       | 1.387 (4)   | C51—H51A      | 0.9500    |
| C4—H4A      | 0.9500      | C53—H53       | 0.9500    |
| C5—C6       | 1.386 (4)   | C54—H54A      | 0.9800    |
| C5—H5A      | 0.9500      | C54—H54B      | 0.9800    |
| C7—C8       | 1.490 (3)   | C54—H54C      | 0.9800    |
| C8—H8A      | 0.9900      | C55—H55A      | 0.9800    |
| C8—H8B      | 0.9900      | C55—H55B      | 0.9800    |
| C9—C10      | 1.498 (3)   | C55—H55C      | 0.9800    |
| C9—H9A      | 0.9900      | C56—H56A      | 0.9500    |
| C9—H9B      | 0.9900      | C57—H57A      | 0.9800    |
| C11—C12     | 1.388 (4)   | C57—H57B      | 0.9800    |
| C11—C16     | 1.396 (4)   | C57—H57C      | 0.9800    |
| C12—C13     | 1.390 (4)   | C58—H58A      | 0.9800    |
| C12—H12A    | 0.9500      | C58—H58B      | 0.9800    |
| C13—C14     | 1.399 (4)   | C58—H58C      | 0.9800    |
| N1—Co—N3    | 140.20 (8)  | N4—C19—H19B   | 109.3     |
| N1—Co—N7    | 99.60 (8)   | C20—C19—H19B  | 109.3     |
| N3—Co—N7    | 100.49 (8)  | H19A—C19—H19B | 107.9     |
| N1—Co—N5    | 97.14 (8)   | C19—C20—H20A  | 109.5     |
| N3—Co—N5    | 85.56 (8)   | C19—C20—H20B  | 109.5     |
| N7—Co—N5    | 144.80 (7)  | H20A—C20—H20B | 109.5     |
| N1—Co—O2    | 103.97 (8)  | C19—C20—H20C  | 109.5     |
| N3—Co—O2    | 114.58 (7)  | H20A—C20—H20C | 109.5     |
| N7—Co—O2    | 73.35 (7)   | H20B—C20—H20C | 109.5     |
| N5—Co—O2    | 72.66 (7)   | N5—C21—C26    | 109.4 (2) |
| N1—Co—O1    | 72.54 (7)   | N5—C21—C22    | 130.8 (2) |
| N3—Co—O1    | 71.85 (7)   | C26—C21—C22   | 119.8 (2) |
| N7—Co—O1    | 94.77 (7)   | C23—C22—C21   | 117.5 (3) |
| N5—Co—O1    | 119.81 (7)  | C23—C22—H22A  | 121.3     |
| O2—Co—O1    | 167.10 (7)  | C21—C22—H22A  | 121.3     |
| C9—O1—C8    | 114.91 (18) | C22—C23—C24   | 122.0 (3) |
| C9—O1—Co    | 120.08 (13) | C22—C23—H23A  | 119.0     |
| C8—O1—Co    | 119.10 (14) | C24—C23—H23A  | 119.0     |
| C29—O2—C28  | 113.99 (18) | C25—C24—C23   | 121.4 (3) |
| C29—O2—Co   | 120.85 (14) | C25—C24—H24A  | 119.3     |
| C28—O2—Co   | 122.57 (15) | C23—C24—H24A  | 119.3     |
| O13—O13—N13 | 0(10)       | C24—C25—C26   | 116.1 (3) |
| O14—O14—N13 | 0(10)       | C24—C25—H25A  | 121.9     |
| C7—N1—C1    | 104.94 (19) | C26—C25—H25A  | 121.9     |
| C7—N1—Co    | 120.31 (17) | N6—C26—C25    | 130.9 (2) |
| C1—N1—Co    | 134.50 (15) | N6—C26—C21    | 105.9 (2) |
| C7—N2—C6    | 106.7 (2)   | C25—C26—C21   | 123.2 (2) |

|             |             |               |             |
|-------------|-------------|---------------|-------------|
| C7—N2—C17   | 125.9 (2)   | N5—C27—N6     | 113.1 (2)   |
| C6—N2—C17   | 127.1 (2)   | N5—C27—C28    | 123.5 (2)   |
| C10—N3—C16  | 105.6 (2)   | N6—C27—C28    | 123.2 (2)   |
| C10—N3—Co   | 120.51 (16) | O2—C28—C27    | 104.38 (19) |
| C16—N3—Co   | 133.02 (16) | O2—C28—H28A   | 110.9       |
| C10—N4—C11  | 106.8 (2)   | C27—C28—H28A  | 110.9       |
| C10—N4—C19  | 125.9 (2)   | O2—C28—H28B   | 110.9       |
| C11—N4—C19  | 127.0 (2)   | C27—C28—H28B  | 110.9       |
| C27—N5—C21  | 105.0 (2)   | H28A—C28—H28B | 108.9       |
| C27—N5—Co   | 116.83 (17) | O2—C29—C30    | 104.42 (19) |
| C21—N5—Co   | 137.15 (16) | O2—C29—H29A   | 110.9       |
| C27—N6—C26  | 106.5 (2)   | C30—C29—H29A  | 110.9       |
| C27—N6—C37  | 126.9 (2)   | O2—C29—H29B   | 110.9       |
| C26—N6—C37  | 126.2 (2)   | C30—C29—H29B  | 110.9       |
| C30—N7—C36  | 105.0 (2)   | H29A—C29—H29B | 108.9       |
| C30—N7—Co   | 117.67 (16) | N7—C30—N8     | 113.7 (2)   |
| C36—N7—Co   | 136.96 (16) | N7—C30—C29    | 122.6 (2)   |
| C30—N8—C31  | 106.5 (2)   | N8—C30—C29    | 123.7 (2)   |
| C30—N8—C39  | 129.1 (2)   | C32—C31—N8    | 131.2 (2)   |
| C31—N8—C39  | 124.2 (2)   | C32—C31—C36   | 122.7 (2)   |
| O5—N9—O4    | 123.9 (3)   | N8—C31—C36    | 106.2 (2)   |
| O5—N9—C42   | 118.2 (4)   | C33—C32—C31   | 116.9 (3)   |
| O4—N9—C42   | 117.9 (3)   | C33—C32—H32A  | 121.5       |
| O6—N10—O7   | 123.9 (3)   | C31—C32—H32A  | 121.5       |
| O6—N10—C44  | 118.3 (3)   | C32—C33—C34   | 121.0 (3)   |
| O7—N10—C44  | 117.9 (3)   | C32—C33—H33A  | 119.5       |
| O9'—N11—O9  | 39.6 (6)    | C34—C33—H33A  | 119.5       |
| O9'—N11—O8  | 79.5 (8)    | C35—C34—C33   | 121.9 (2)   |
| O9—N11—O8   | 113.3 (6)   | C35—C34—H34A  | 119.0       |
| O9'—N11—O8' | 123.6 (8)   | C33—C34—H34A  | 119.0       |
| O9—N11—O8'  | 105.6 (6)   | C34—C35—C36   | 117.4 (2)   |
| O8—N11—O8'  | 84.5 (5)    | C34—C35—H35A  | 121.3       |
| O9'—N11—C46 | 119.3 (7)   | C36—C35—H35A  | 121.3       |
| O9—N11—C46  | 117.2 (5)   | C35—C36—C31   | 120.1 (2)   |
| O8—N11—C46  | 115.1 (4)   | C35—C36—N7    | 131.4 (2)   |
| O8'—N11—C46 | 116.5 (4)   | C31—C36—N7    | 108.6 (2)   |
| O11—N12—O12 | 123.9 (2)   | N6—C37—C38    | 111.9 (2)   |
| O11—N12—C48 | 118.1 (2)   | N6—C37—H37A   | 109.2       |
| O12—N12—C48 | 118.0 (2)   | C38—C37—H37A  | 109.2       |
| O13—N13—O13 | 0.0 (2)     | N6—C37—H37B   | 109.2       |
| O13—N13—O14 | 122.8 (2)   | C38—C37—H37B  | 109.2       |
| O13—N13—O14 | 122.8 (2)   | H37A—C37—H37B | 107.9       |
| O13—N13—O14 | 122.8 (2)   | C37—C38—H38A  | 109.5       |
| O13—N13—O14 | 122.8 (2)   | C37—C38—H38B  | 109.5       |
| O14—N13—O14 | 0.00 (19)   | H38A—C38—H38B | 109.5       |
| O13—N13—C50 | 118.6 (2)   | C37—C38—H38C  | 109.5       |
| O13—N13—C50 | 118.6 (2)   | H38A—C38—H38C | 109.5       |
| O14—N13—C50 | 118.6 (2)   | H38B—C38—H38C | 109.5       |
| O14—N13—C50 | 118.6 (2)   | N8—C39—C40    | 111.6 (2)   |

## supplementary materials

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|             |             |               |           |
|-------------|-------------|---------------|-----------|
| O15—N14—O16 | 123.0 (3)   | N8—C39—H39A   | 109.3     |
| O15—N14—C52 | 118.2 (2)   | C40—C39—H39A  | 109.3     |
| O16—N14—C52 | 118.7 (2)   | N8—C39—H39B   | 109.3     |
| C53—N15—C54 | 120.6 (3)   | C40—C39—H39B  | 109.3     |
| C53—N15—C55 | 124.2 (4)   | H39A—C39—H39B | 108.0     |
| C54—N15—C55 | 115.0 (3)   | C39—C40—H40A  | 109.5     |
| C56—N16—C58 | 122.2 (3)   | C39—C40—H40B  | 109.5     |
| C56—N16—C57 | 120.8 (3)   | H40A—C40—H40B | 109.5     |
| C58—N16—C57 | 116.8 (3)   | C39—C40—H40C  | 109.5     |
| N1—C1—C2    | 130.4 (2)   | H40A—C40—H40C | 109.5     |
| N1—C1—C6    | 109.3 (2)   | H40B—C40—H40C | 109.5     |
| C2—C1—C6    | 120.3 (2)   | O3—C41—C46    | 124.5 (3) |
| C3—C2—C1    | 117.4 (2)   | O3—C41—C42    | 125.1 (3) |
| C3—C2—H2A   | 121.3       | C46—C41—C42   | 110.4 (2) |
| C1—C2—H2A   | 121.3       | C43—C42—C41   | 124.9 (3) |
| C2—C3—C4    | 122.0 (2)   | C43—C42—N9    | 116.5 (3) |
| C2—C3—H3A   | 119.0       | C41—C42—N9    | 118.5 (3) |
| C4—C3—H3A   | 119.0       | C42—C43—C44   | 119.5 (3) |
| C5—C4—C3    | 121.2 (3)   | C42—C43—H43A  | 120.2     |
| C5—C4—H4A   | 119.4       | C44—C43—H43A  | 120.2     |
| C3—C4—H4A   | 119.4       | C45—C44—C43   | 120.3 (3) |
| C6—C5—C4    | 116.6 (2)   | C45—C44—N10   | 119.5 (3) |
| C6—C5—H5A   | 121.7       | C43—C44—N10   | 120.1 (3) |
| C4—C5—H5A   | 121.7       | C46—C45—C44   | 119.8 (3) |
| C5—C6—N2    | 131.9 (2)   | C46—C45—H45A  | 120.1     |
| C5—C6—C1    | 122.6 (2)   | C44—C45—H45A  | 120.1     |
| N2—C6—C1    | 105.6 (2)   | C45—C46—C41   | 125.0 (3) |
| N1—C7—N2    | 113.5 (2)   | C45—C46—N11   | 113.4 (3) |
| N1—C7—C8    | 122.8 (2)   | C41—C46—N11   | 121.6 (3) |
| N2—C7—C8    | 123.7 (2)   | O10—C47—C48   | 124.0 (2) |
| O1—C8—C7    | 104.67 (18) | O10—C47—C52   | 125.0 (3) |
| O1—C8—H8A   | 110.8       | C48—C47—C52   | 110.9 (2) |
| C7—C8—H8A   | 110.8       | C49—C48—C47   | 125.3 (2) |
| O1—C8—H8B   | 110.8       | C49—C48—N12   | 117.3 (2) |
| C7—C8—H8B   | 110.8       | C47—C48—N12   | 117.3 (2) |
| H8A—C8—H8B  | 108.9       | C48—C49—C50   | 118.7 (3) |
| O1—C9—C10   | 104.92 (19) | C48—C49—H49A  | 120.6     |
| O1—C9—H9A   | 110.8       | C50—C49—H49A  | 120.6     |
| C10—C9—H9A  | 110.8       | C51—C50—C49   | 120.9 (2) |
| O1—C9—H9B   | 110.8       | C51—C50—N13   | 120.1 (2) |
| C10—C9—H9B  | 110.8       | C49—C50—N13   | 119.0 (2) |
| H9A—C9—H9B  | 108.8       | C52—C51—C50   | 119.4 (2) |
| N3—C10—N4   | 112.9 (2)   | C52—C51—H51A  | 120.3     |
| N3—C10—C9   | 122.2 (2)   | C50—C51—H51A  | 120.3     |
| N4—C10—C9   | 124.8 (2)   | C51—C52—N14   | 117.7 (2) |
| C12—C11—N4  | 131.8 (2)   | C51—C52—C47   | 124.4 (3) |
| C12—C11—C16 | 122.3 (2)   | N14—C52—C47   | 117.8 (2) |
| N4—C11—C16  | 105.9 (2)   | O17—C53—N15   | 127.5 (4) |
| C11—C12—C13 | 116.0 (3)   | O17—C53—H53   | 116.3     |

|               |              |                 |              |
|---------------|--------------|-----------------|--------------|
| C11—C12—H12A  | 122.0        | N15—C53—H53     | 116.3        |
| C13—C12—H12A  | 122.0        | N15—C54—H54A    | 109.5        |
| C12—C13—C14   | 122.2 (2)    | N15—C54—H54B    | 109.5        |
| C12—C13—H13A  | 118.9        | H54A—C54—H54B   | 109.5        |
| C14—C13—H13A  | 118.9        | N15—C54—H54C    | 109.5        |
| C15—C14—C13   | 121.2 (2)    | H54A—C54—H54C   | 109.5        |
| C15—C14—H14A  | 119.4        | H54B—C54—H54C   | 109.5        |
| C13—C14—H14A  | 119.4        | N15—C55—H55A    | 109.5        |
| C14—C15—C16   | 117.4 (3)    | N15—C55—H55B    | 109.5        |
| C14—C15—H15A  | 121.3        | H55A—C55—H55B   | 109.5        |
| C16—C15—H15A  | 121.3        | N15—C55—H55C    | 109.5        |
| C15—C16—N3    | 130.4 (2)    | H55A—C55—H55C   | 109.5        |
| C15—C16—C11   | 120.9 (2)    | H55B—C55—H55C   | 109.5        |
| N3—C16—C11    | 108.7 (2)    | O18—C56—N16     | 126.1 (3)    |
| N2—C17—C18    | 112.7 (2)    | O18—C56—H56A    | 117.0        |
| N2—C17—H17A   | 109.0        | N16—C56—H56A    | 117.0        |
| C18—C17—H17A  | 109.0        | N16—C57—H57A    | 109.5        |
| N2—C17—H17B   | 109.0        | N16—C57—H57B    | 109.5        |
| C18—C17—H17B  | 109.0        | H57A—C57—H57B   | 109.5        |
| H17A—C17—H17B | 107.8        | N16—C57—H57C    | 109.5        |
| C17—C18—H18A  | 109.5        | H57A—C57—H57C   | 109.5        |
| C17—C18—H18B  | 109.5        | H57B—C57—H57C   | 109.5        |
| H18A—C18—H18B | 109.5        | N16—C58—H58A    | 109.5        |
| C17—C18—H18C  | 109.5        | N16—C58—H58B    | 109.5        |
| H18A—C18—H18C | 109.5        | H58A—C58—H58B   | 109.5        |
| H18B—C18—H18C | 109.5        | N16—C58—H58C    | 109.5        |
| N4—C19—C20    | 111.7 (2)    | H58A—C58—H58C   | 109.5        |
| N4—C19—H19A   | 109.3        | H58B—C58—H58C   | 109.5        |
| C20—C19—H19A  | 109.3        |                 |              |
| N1—Co—O1—C9   | -155.93 (19) | Co—N5—C21—C26   | 168.72 (18)  |
| N3—Co—O1—C9   | 6.00 (17)    | C27—N5—C21—C22  | -178.8 (3)   |
| N7—Co—O1—C9   | 105.49 (18)  | Co—N5—C21—C22   | -11.2 (4)    |
| N5—Co—O1—C9   | -67.64 (19)  | N5—C21—C22—C23  | -179.5 (3)   |
| O2—Co—O1—C9   | 128.0 (3)    | C26—C21—C22—C23 | 0.6 (4)      |
| N1—Co—O1—C8   | -4.36 (17)   | C21—C22—C23—C24 | -0.6 (4)     |
| N3—Co—O1—C8   | 157.56 (18)  | C22—C23—C24—C25 | 0.0 (5)      |
| N7—Co—O1—C8   | -102.94 (17) | C23—C24—C25—C26 | 0.4 (4)      |
| N5—Co—O1—C8   | 83.92 (18)   | C27—N6—C26—C25  | 179.1 (3)    |
| O2—Co—O1—C8   | -80.5 (4)    | C37—N6—C26—C25  | 5.1 (5)      |
| N1—Co—O2—C29  | -106.16 (18) | C27—N6—C26—C21  | -0.6 (3)     |
| N3—Co—O2—C29  | 84.01 (19)   | C37—N6—C26—C21  | -174.5 (2)   |
| N7—Co—O2—C29  | -10.14 (17)  | C24—C25—C26—N6  | 179.9 (3)    |
| N5—Co—O2—C29  | 160.60 (19)  | C24—C25—C26—C21 | -0.4 (4)     |
| O1—Co—O2—C29  | -33.6 (4)    | N5—C21—C26—N6   | -0.3 (3)     |
| N1—Co—O2—C28  | 93.21 (19)   | C22—C21—C26—N6  | 179.6 (2)    |
| N3—Co—O2—C28  | -76.6 (2)    | N5—C21—C26—C25  | 180.0 (2)    |
| N7—Co—O2—C28  | -170.8 (2)   | C22—C21—C26—C25 | -0.1 (4)     |
| N5—Co—O2—C28  | -0.04 (18)   | C21—N5—C27—N6   | -1.6 (3)     |
| O1—Co—O2—C28  | 165.8 (3)    | Co—N5—C27—N6    | -172.15 (16) |

## supplementary materials

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|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| N3—Co—N1—C7     | -28.3 (2)    | C21—N5—C27—C28  | 174.0 (2)    |
| N7—Co—N1—C7     | 91.11 (19)   | Co—N5—C27—C28   | 3.5 (3)      |
| N5—Co—N1—C7     | -119.97 (18) | C26—N6—C27—N5   | 1.4 (3)      |
| O2—Co—N1—C7     | 166.19 (18)  | C37—N6—C27—N5   | 175.3 (2)    |
| O1—Co—N1—C7     | -0.91 (17)   | C26—N6—C27—C28  | -174.2 (2)   |
| N3—Co—N1—C1     | 158.5 (2)    | C37—N6—C27—C28  | -0.3 (4)     |
| N7—Co—N1—C1     | -82.1 (2)    | C29—O2—C28—C27  | -160.4 (2)   |
| N5—Co—N1—C1     | 66.8 (2)     | Co—O2—C28—C27   | 1.5 (3)      |
| O2—Co—N1—C1     | -7.0 (2)     | N5—C27—C28—O2   | -3.2 (3)     |
| O1—Co—N1—C1     | -174.1 (2)   | N6—C27—C28—O2   | 172.0 (2)    |
| N1—Co—N3—C10    | 21.8 (3)     | C28—O2—C29—C30  | 171.8 (2)    |
| N7—Co—N3—C10    | -97.34 (19)  | Co—O2—C29—C30   | 9.6 (3)      |
| N5—Co—N3—C10    | 117.65 (19)  | C36—N7—C30—N8   | -0.1 (3)     |
| O2—Co—N3—C10    | -173.70 (17) | Co—N7—C30—N8    | 174.38 (16)  |
| O1—Co—N3—C10    | -5.72 (18)   | C36—N7—C30—C29  | 179.7 (2)    |
| N1—Co—N3—C16    | -146.1 (2)   | Co—N7—C30—C29   | -5.9 (3)     |
| N7—Co—N3—C16    | 94.8 (2)     | C31—N8—C30—N7   | -0.6 (3)     |
| N5—Co—N3—C16    | -50.2 (2)    | C39—N8—C30—N7   | -175.7 (2)   |
| O2—Co—N3—C16    | 18.4 (2)     | C31—N8—C30—C29  | 179.6 (2)    |
| O1—Co—N3—C16    | -173.6 (2)   | C39—N8—C30—C29  | 4.5 (4)      |
| N1—Co—N5—C27    | -104.17 (18) | O2—C29—C30—N7   | -2.4 (3)     |
| N3—Co—N5—C27    | 115.76 (18)  | O2—C29—C30—N8   | 177.3 (2)    |
| N7—Co—N5—C27    | 13.8 (3)     | C30—N8—C31—C32  | -179.7 (3)   |
| O2—Co—N5—C27    | -1.72 (17)   | C39—N8—C31—C32  | -4.2 (4)     |
| O1—Co—N5—C27    | -178.11 (16) | C30—N8—C31—C36  | 1.1 (3)      |
| N1—Co—N5—C21    | 89.3 (2)     | C39—N8—C31—C36  | 176.5 (2)    |
| N3—Co—N5—C21    | -50.8 (2)    | N8—C31—C32—C33  | -178.2 (3)   |
| N7—Co—N5—C21    | -152.7 (2)   | C36—C31—C32—C33 | 0.9 (4)      |
| O2—Co—N5—C21    | -168.3 (2)   | C31—C32—C33—C34 | 0.1 (4)      |
| O1—Co—N5—C21    | 15.3 (3)     | C32—C33—C34—C35 | -0.1 (4)     |
| N1—Co—N7—C30    | 109.79 (18)  | C33—C34—C35—C36 | -0.8 (4)     |
| N3—Co—N7—C30    | -104.75 (18) | C34—C35—C36—C31 | 1.7 (4)      |
| N5—Co—N7—C30    | -7.5 (3)     | C34—C35—C36—N7  | -179.9 (3)   |
| O2—Co—N7—C30    | 7.96 (17)    | C32—C31—C36—C35 | -1.9 (4)     |
| O1—Co—N7—C30    | -177.14 (17) | N8—C31—C36—C35  | 177.5 (2)    |
| N1—Co—N7—C36    | -78.0 (2)    | C32—C31—C36—N7  | 179.5 (2)    |
| N3—Co—N7—C36    | 67.5 (2)     | N8—C31—C36—N7   | -1.2 (3)     |
| N5—Co—N7—C36    | 164.7 (2)    | C30—N7—C36—C35  | -177.6 (3)   |
| O2—Co—N7—C36    | -179.8 (2)   | Co—N7—C36—C35   | 9.5 (4)      |
| O1—Co—N7—C36    | -4.9 (2)     | C30—N7—C36—C31  | 0.8 (3)      |
| O13—O13—N13—O14 | 0.00 (19)    | Co—N7—C36—C31   | -172.02 (18) |
| O13—O13—N13—O14 | 0.00 (19)    | C27—N6—C37—C38  | -95.6 (3)    |
| O13—O13—N13—C50 | 0.00 (14)    | C26—N6—C37—C38  | 77.1 (3)     |
| O14—O14—N13—O13 | 0.00 (10)    | C30—N8—C39—C40  | 101.1 (3)    |
| O14—O14—N13—O13 | 0.00 (10)    | C31—N8—C39—C40  | -73.2 (3)    |
| O14—O14—N13—C50 | 0.00 (15)    | O3—C41—C42—C43  | 175.2 (3)    |
| C7—N1—C1—C2     | 178.0 (3)    | C46—C41—C42—C43 | -1.8 (4)     |
| Co—N1—C1—C2     | -8.1 (4)     | O3—C41—C42—N9   | -1.4 (5)     |
| C7—N1—C1—C6     | -0.5 (3)     | C46—C41—C42—N9  | -178.4 (3)   |

|                 |              |                 |            |
|-----------------|--------------|-----------------|------------|
| Co—N1—C1—C6     | 173.48 (17)  | O5—N9—C42—C43   | 142.6 (3)  |
| N1—C1—C2—C3     | 179.9 (2)    | O4—N9—C42—C43   | -37.0 (4)  |
| C6—C1—C2—C3     | -1.9 (4)     | O5—N9—C42—C41   | -40.5 (4)  |
| C1—C2—C3—C4     | 0.7 (4)      | O4—N9—C42—C41   | 139.9 (3)  |
| C2—C3—C4—C5     | 0.6 (4)      | C41—C42—C43—C44 | 3.3 (4)    |
| C3—C4—C5—C6     | -0.7 (4)     | N9—C42—C43—C44  | 180.0 (3)  |
| C4—C5—C6—N2     | 179.2 (3)    | C42—C43—C44—C45 | -2.9 (4)   |
| C4—C5—C6—C1     | -0.5 (4)     | C42—C43—C44—N10 | -178.8 (2) |
| C7—N2—C6—C5     | 179.6 (3)    | O6—N10—C44—C45  | 179.9 (3)  |
| C17—N2—C6—C5    | -6.3 (4)     | O7—N10—C44—C45  | -0.9 (4)   |
| C7—N2—C6—C1     | -0.6 (3)     | O6—N10—C44—C43  | -4.2 (4)   |
| C17—N2—C6—C1    | 173.5 (2)    | O7—N10—C44—C43  | 175.0 (2)  |
| N1—C1—C6—C5     | -179.5 (2)   | C43—C44—C45—C46 | 1.1 (4)    |
| C2—C1—C6—C5     | 1.9 (4)      | N10—C44—C45—C46 | 177.0 (3)  |
| N1—C1—C6—N2     | 0.7 (3)      | C44—C45—C46—C41 | 0.4 (5)    |
| C2—C1—C6—N2     | -177.9 (2)   | C44—C45—C46—N11 | -176.1 (3) |
| C1—N1—C7—N2     | 0.0 (3)      | O3—C41—C46—C45  | -177.1 (3) |
| Co—N1—C7—N2     | -174.95 (16) | C42—C41—C46—C45 | -0.1 (4)   |
| C1—N1—C7—C8     | -178.9 (2)   | O3—C41—C46—N11  | -0.9 (5)   |
| Co—N1—C7—C8     | 6.1 (3)      | C42—C41—C46—N11 | 176.1 (3)  |
| C6—N2—C7—N1     | 0.4 (3)      | O9'—N11—C46—C45 | -150.0 (9) |
| C17—N2—C7—N1    | -173.8 (2)   | O9—N11—C46—C45  | 164.8 (6)  |
| C6—N2—C7—C8     | 179.3 (2)    | O8—N11—C46—C45  | -58.3 (6)  |
| C17—N2—C7—C8    | 5.1 (4)      | O8'—N11—C46—C45 | 38.4 (5)   |
| C9—O1—C8—C7     | 160.6 (2)    | O9'—N11—C46—C41 | 33.4 (10)  |
| Co—O1—C8—C7     | 7.6 (2)      | O9—N11—C46—C41  | -11.7 (7)  |
| N1—C7—C8—O1     | -8.8 (3)     | O8—N11—C46—C41  | 125.2 (5)  |
| N2—C7—C8—O1     | 172.4 (2)    | O8'—N11—C46—C41 | -138.2 (5) |
| C8—O1—C9—C10    | -157.7 (2)   | O10—C47—C48—C49 | 169.2 (3)  |
| Co—O1—C9—C10    | -5.0 (2)     | C52—C47—C48—C49 | -6.8 (4)   |
| C16—N3—C10—N4   | -1.1 (3)     | O10—C47—C48—N12 | -7.7 (4)   |
| Co—N3—C10—N4    | -171.93 (16) | C52—C47—C48—N12 | 176.3 (2)  |
| C16—N3—C10—C9   | 176.2 (2)    | O11—N12—C48—C49 | 140.6 (3)  |
| Co—N3—C10—C9    | 5.4 (3)      | O12—N12—C48—C49 | -39.2 (4)  |
| C11—N4—C10—N3   | 1.3 (3)      | O11—N12—C48—C47 | -42.2 (4)  |
| C19—N4—C10—N3   | 175.7 (2)    | O12—N12—C48—C47 | 138.0 (3)  |
| C11—N4—C10—C9   | -176.0 (2)   | C47—C48—C49—C50 | 4.0 (4)    |
| C19—N4—C10—C9   | -1.5 (4)     | N12—C48—C49—C50 | -179.1 (2) |
| O1—C9—C10—N3    | 0.0 (3)      | C48—C49—C50—C51 | 0.0 (4)    |
| O1—C9—C10—N4    | 177.0 (2)    | C48—C49—C50—N13 | 179.5 (2)  |
| C10—N4—C11—C12  | 178.7 (3)    | O13—N13—C50—C51 | -178.5 (3) |
| C19—N4—C11—C12  | 4.3 (4)      | O13—N13—C50—C51 | -178.5 (3) |
| C10—N4—C11—C16  | -0.9 (3)     | O14—N13—C50—C51 | 0.6 (4)    |
| C19—N4—C11—C16  | -175.3 (2)   | O14—N13—C50—C51 | 0.6 (4)    |
| N4—C11—C12—C13  | -179.5 (3)   | O13—N13—C50—C49 | 1.9 (4)    |
| C16—C11—C12—C13 | 0.1 (4)      | O13—N13—C50—C49 | 1.9 (4)    |
| C11—C12—C13—C14 | -0.2 (4)     | O14—N13—C50—C49 | -178.9 (2) |
| C12—C13—C14—C15 | 0.1 (5)      | O14—N13—C50—C49 | -178.9 (2) |
| C13—C14—C15—C16 | 0.3 (4)      | C49—C50—C51—C52 | -0.3 (4)   |

## supplementary materials

|                 |             |                 |            |
|-----------------|-------------|-----------------|------------|
| C14—C15—C16—N3  | 179.1 (3)   | N13—C50—C51—C52 | -179.8 (3) |
| C14—C15—C16—C11 | -0.5 (4)    | C50—C51—C52—N14 | -179.9 (3) |
| C10—N3—C16—C15  | -179.2 (3)  | C50—C51—C52—C47 | -3.3 (4)   |
| Co—N3—C16—C15   | -10.0 (4)   | O15—N14—C52—C51 | 33.4 (4)   |
| C10—N3—C16—C11  | 0.5 (3)     | O16—N14—C52—C51 | -145.2 (3) |
| Co—N3—C16—C11   | 169.68 (17) | O15—N14—C52—C47 | -143.4 (3) |
| C12—C11—C16—C15 | 0.3 (4)     | O16—N14—C52—C47 | 38.0 (4)   |
| N4—C11—C16—C15  | 180.0 (2)   | O10—C47—C52—C51 | -169.6 (3) |
| C12—C11—C16—N3  | -179.4 (2)  | C48—C47—C52—C51 | 6.4 (4)    |
| N4—C11—C16—N3   | 0.2 (3)     | O10—C47—C52—N14 | 7.0 (4)    |
| C7—N2—C17—C18   | -110.1 (3)  | C48—C47—C52—N14 | -177.0 (2) |
| C6—N2—C17—C18   | 76.9 (3)    | C54—N15—C53—O17 | -1.8 (9)   |
| C10—N4—C19—C20  | -86.1 (3)   | C55—N15—C53—O17 | -176.0 (7) |
| C11—N4—C19—C20  | 87.2 (3)    | C58—N16—C56—O18 | -176.6 (4) |
| C27—N5—C21—C26  | 1.1 (3)     | C57—N16—C56—O18 | -1.4 (5)   |

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

| <i>D</i> —H $\cdots$ <i>A</i>        | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|--------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C18—H18B $\cdots$ O12 <sup>i</sup>   | 0.98        | 2.57                | 3.342 (4)                  | 135                           |
| C15—H15A $\cdots$ O13                | 0.95        | 2.56                | 3.191 (3)                  | 124                           |
| C18—H18B $\cdots$ O12 <sup>i</sup>   | 0.98        | 2.57                | 3.342 (4)                  | 135                           |
| C28—H28A $\cdots$ O17 <sup>ii</sup>  | 0.99        | 2.38                | 3.365 (4)                  | 173                           |
| C28—H28B $\cdots$ O10 <sup>iii</sup> | 0.99        | 2.29                | 2.994 (3)                  | 128                           |
| C29—H29A $\cdots$ O14                | 0.99        | 2.39                | 3.331 (3)                  | 158                           |
| C35—H35A $\cdots$ O7 <sup>i</sup>    | 0.95        | 2.44                | 3.158 (3)                  | 133                           |
| C53—H53 $\cdots$ O9 <sup>iv</sup>    | 0.95        | 2.39                | 3.242 (7)                  | 148                           |
| C56—H56A $\cdots$ O3 <sup>v</sup>    | 0.95        | 2.46                | 3.335 (4)                  | 154                           |

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

Fig. 1

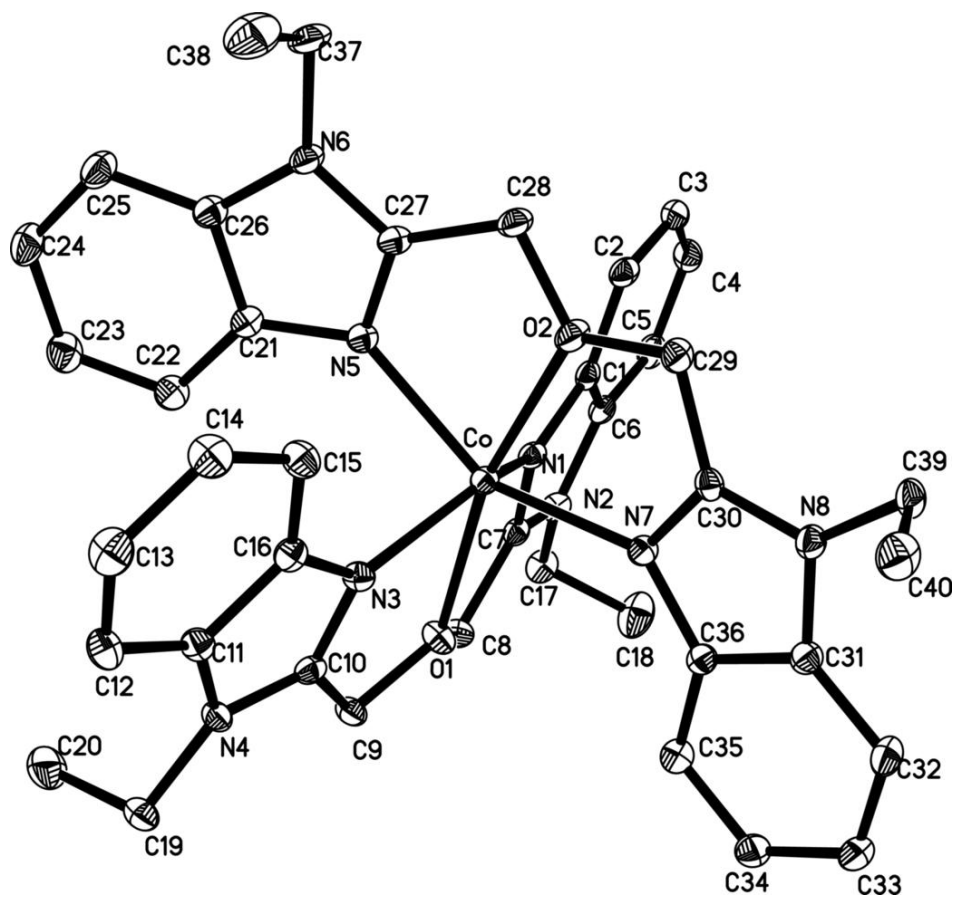


Fig. 2

