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Bis[1-(1-adamantyliminomethyl)-2-naphtholato- $\kappa^2N,O$ ]cobalt(II)

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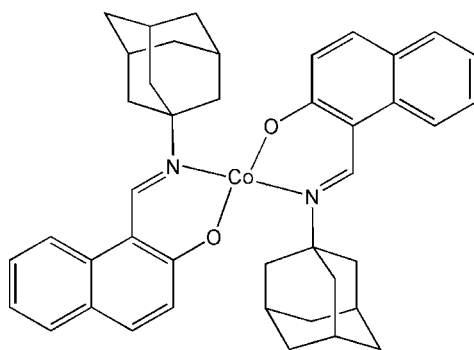
Received 8 August 2008; accepted 26 August 2008

Key indicators: single-crystal X-ray study;  $T = 90$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.088; data-to-parameter ratio = 18.0.

The title compound,  $[Co(C_{21}H_{22}NO)_2]$ , crystallizes with two molecules in the asymmetric unit. The coordination environments of the two  $Co^{II}$  ions are distorted tetrahedral. The primary structural difference between the two independent complex molecules lies in the orientations of their adamantyl groups.

## Related literature

For structures of the ligand and a copper complex of the ligand, see: Acevedo-Arauz *et al.* (1992). For a carboxylato-bridged Rh dimer with axial coordination of the neutral ligand, see: Franco *et al.* (2007).



## Experimental

## Crystal data

 $[Co(C_{21}H_{22}NO)_2]$  $M_r = 667.72$ 

Triclinic,  $P\bar{1}$   
 $a = 13.9055$  (5) Å  
 $b = 14.3576$  (5) Å  
 $c = 19.5899$  (6) Å  
 $\alpha = 69.938$  (2)°  
 $\beta = 71.219$  (2)°  
 $\gamma = 68.473$  (2)°

$V = 3330.4$  (2) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.56$  mm<sup>-1</sup>  
 $T = 90$  (2) K  
 $0.33 \times 0.24 \times 0.18$  mm

## Data collection

Bruker SMART APEXII diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.876$ ,  $T_{\max} = 0.925$

42959 measured reflections  
 15246 independent reflections  
 11999 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.088$   
 $S = 1.02$   
 15246 reflections

847 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.32$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

|           |             |           |             |
|-----------|-------------|-----------|-------------|
| Co1—O1    | 1.9051 (12) | Co2—O3    | 1.9139 (12) |
| Co1—O2    | 1.9192 (12) | Co2—O4    | 1.9194 (12) |
| Co1—N1    | 1.9962 (14) | Co2—N3    | 1.9945 (13) |
| Co1—N2    | 2.0019 (14) | Co2—N4    | 1.9849 (14) |
| O1—Co1—O2 | 115.23 (5)  | O3—Co2—O4 | 114.40 (5)  |
| O1—Co1—N1 | 94.93 (5)   | O3—Co2—N3 | 94.94 (5)   |
| O2—Co1—N1 | 117.15 (5)  | O3—Co2—N4 | 116.97 (5)  |
| O1—Co1—N2 | 115.95 (5)  | O4—Co2—N3 | 115.20 (5)  |
| O2—Co1—N2 | 93.16 (5)   | O4—Co2—N4 | 94.63 (5)   |
| N1—Co1—N2 | 122.20 (6)  | N3—Co2—N4 | 122.25 (6)  |

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: SHELXL97.

The authors thank the University of California, Davis, for acquisition of the Bruker SMART APEXII diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2163).

## References

- Acevedo-Arauz, E., Fernández-G, J. M., Rosales-Hoz, M. J. & Toscano, R. A. (1992). *Acta Cryst.* **C48**, 115–120.  
 Bruker (2007). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Franco, J. U., Olmstead, M. M. & Hammons, J. C. (2007). *Acta Cryst.* **E63**, m2606–m2607.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

**supplementary materials**

*Acta Cryst.* (2008). E64, m1223 [ doi:10.1107/S1600536808027475 ]

## Bis[1-(1-adamantyliminomethyl)-2-naphtholato- $\kappa^2N,O$ ]cobalt(II)

J. U. Franco, M. M. Olmstead and J. C. Hammons

### Comment

The title  $\text{Co}^{\text{II}}$  complex has two bidentate Schiff base ligands in a typical coordination mode involving N and O donor atoms. A similar bidentate mode of coordination for the same ligand has been reported in the bis- $\text{Cu}^{\text{II}}$  complex (Acevedo-Arauz *et al.*, 1992). Earlier (Franco *et al.*, 2007), we reported the structure of a carboxylato-bridged Rh dimer in which the neutral ligand binds axially in a monodentate mode through the oxygen atom and forms an intramolecular hydrogen bond to the N atom. The bidentate coordination mode of the title complex is fundamentally different because the ligand has been deprotonated.

There are two molecules in the asymmetric unit. These are depicted in Fig. 1 as they occur in the structure. The coordination geometry for  $\text{Co}^{\text{II}}$  is in the normal range for complexes of this type. The  $\text{N}_2\text{O}_2$  donor set forms a distorted tetrahedral coordination with angles at Co ranging from 93.16 (5) $^\circ$  to 122.20 (6) $^\circ$  in the complex involving Co1 and 94.63 (5) $^\circ$  to 122.25 (6) $^\circ$  in the complex involving Co2. A calculation of the least-squares plane of the thirteen atoms comprising the 2-naphthol-iminomethyl ligand reveals a marked deviation from planarity at the imino carbon atom. An inspection of the structure indicates that this buckling is likely due to a short intramolecular contact between the C—H hydrogen and one of the naphthol H atoms. The deviations of this carbon from the four different ligand planes are 0.1146 (13) Å, C11; 0.1861 (14) Å, C32; 0.0992 (14) Å, C53; 0.1223 (14) Å, C74.

In addition to these differences in buckling of the Schiff base, the two molecules differ in the rotation of the adamantyl substituent. These are attributable to packing interactions.

### Experimental

The ligand, 1-(1-adamantyl)iminomethyl)-2-naphthol, was prepared as previously described (Franco *et al.*, 2007). The Co complex was prepared as follows. In a 100 ml round bottom flask, 50 mg of 1-(1-adamantyl)iminomethyl)-2-naphthol (16 mmol) was dissolved in 30 ml of methanol, followed by addition of 7 mg of methanolic NaOH (16 mmol). After the solution was stirred for ten minutes, 16 mg of  $\text{CoCl}_2 \cdot 2(\text{H}_2\text{O})$  (8 mmol) dissolved in 15 ml of methanol was added and the reaction mixture stirred for another three hours at room temperature. The solution was then filtered to remove any solids and the solvent removed by use of a rotary evaporator. The residue was crystallized by slow evaporation of a methanol solution to afford red-orange crystals, yield 84%.

### Refinement

The C-bound H atoms were positioned geometrically with C—H = 0.95–0.99 Å, and allowed to ride on their parent atoms with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

## Figures

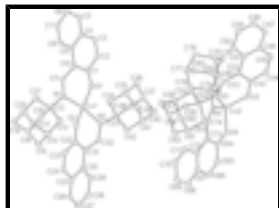


Fig. 1. A view of both molecules in the asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

## Bis[1-(1-adamantyliminomethyl)-2-naphtholato- $\kappa^2N,O$ ]cobalt(II)

### Crystal data

[Co(C<sub>21</sub>H<sub>22</sub>NO)<sub>2</sub>]

$M_r = 667.72$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 13.9055$  (5) Å

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$c = 19.5899$  (6) Å

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$\beta = 71.219$  (2)°

$\gamma = 68.473$  (2)°

$V = 3330.4$  (2) Å<sup>3</sup>

$Z = 4$

$F_{000} = 1412$

$D_x = 1.332$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 5583 reflections

$\theta = 2.8$ – $27.4$ °

$\mu = 0.56$  mm<sup>-1</sup>

$T = 90$  (2) K

Plate, red-orange

$0.33 \times 0.24 \times 0.18$  mm

### Data collection

Bruker SMART APEXII  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.3 pixels mm<sup>-1</sup>

$T = 90$ (2) K

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.876$ ,  $T_{\max} = 0.925$

42959 measured reflections

15246 independent reflections

11999 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 2.8$ °

$h = -18 \rightarrow 18$

$k = -18 \rightarrow 18$

$l = -25 \rightarrow 25$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.036$

$wR(F^2) = 0.088$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.0354P]$

$S = 1.02$   
 15246 reflections  
 847 parameters  
 Primary atom site location: structure-invariant direct methods  
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$   
 Extinction correction: none

*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>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|---------------|----------------------------------|
| Co1  | 0.588500 (17) | 0.756438 (17) | 0.086566 (12) | 0.01448 (6)                      |
| O2   | 0.44739 (9)   | 0.80539 (9)   | 0.14274 (7)   | 0.0199 (3)                       |
| O1   | 0.69699 (9)   | 0.78062 (9)   | 0.11194 (6)   | 0.0191 (3)                       |
| N1   | 0.62251 (11)  | 0.83082 (10)  | -0.02092 (8)  | 0.0142 (3)                       |
| N2   | 0.58369 (11)  | 0.60961 (11)  | 0.11945 (8)   | 0.0148 (3)                       |
| C1   | 0.77555 (13)  | 0.81402 (13)  | 0.06543 (9)   | 0.0165 (3)                       |
| C2   | 0.85436 (14)  | 0.81505 (14)  | 0.09778 (10)  | 0.0200 (4)                       |
| H2   | 0.8472        | 0.7904        | 0.1503        | 0.024*                           |
| C3   | 0.93834 (14)  | 0.85025 (13)  | 0.05544 (10)  | 0.0196 (4)                       |
| H3   | 0.9875        | 0.8518        | 0.0790        | 0.024*                           |
| C4   | 0.95482 (13)  | 0.88506 (13)  | -0.02376 (10) | 0.0173 (3)                       |
| C5   | 1.04467 (14)  | 0.91845 (13)  | -0.06732 (10) | 0.0205 (4)                       |
| H5   | 1.0930        | 0.9203        | -0.0432       | 0.025*                           |
| C6   | 1.06366 (14)  | 0.94821 (14)  | -0.14352 (11) | 0.0222 (4)                       |
| H6   | 1.1239        | 0.9715        | -0.1721       | 0.027*                           |
| C7   | 0.99276 (14)  | 0.94382 (13)  | -0.17891 (10) | 0.0203 (4)                       |
| H7   | 1.0059        | 0.9632        | -0.2318       | 0.024*                           |
| C8   | 0.90448 (13)  | 0.91185 (13)  | -0.13780 (10) | 0.0175 (3)                       |
| H8   | 0.8583        | 0.9088        | -0.1631       | 0.021*                           |
| C9   | 0.88031 (13)  | 0.88328 (12)  | -0.05871 (9)  | 0.0154 (3)                       |
| C10  | 0.78698 (13)  | 0.85024 (12)  | -0.01287 (9)  | 0.0150 (3)                       |
| C11  | 0.70689 (13)  | 0.86179 (12)  | -0.04951 (9)  | 0.0149 (3)                       |
| H11  | 0.7173        | 0.8965        | -0.1011       | 0.018*                           |
| C12  | 0.54877 (13)  | 0.85018 (13)  | -0.06884 (9)  | 0.0155 (3)                       |
| C13  | 0.54044 (14)  | 0.74344 (13)  | -0.06166 (10) | 0.0201 (4)                       |
| H13A | 0.6107        | 0.6999        | -0.0824       | 0.024*                           |

## supplementary materials

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|      |              |              |               |            |
|------|--------------|--------------|---------------|------------|
| H13B | 0.5188       | 0.7089       | -0.0083       | 0.024*     |
| C14  | 0.45935 (15) | 0.75395 (15) | -0.10333 (11) | 0.0246 (4) |
| H14  | 0.4550       | 0.6838       | -0.0981       | 0.029*     |
| C15  | 0.35098 (15) | 0.81967 (16) | -0.06975 (11) | 0.0269 (4) |
| H15A | 0.3291       | 0.7860       | -0.0162       | 0.032*     |
| H15B | 0.2973       | 0.8257       | -0.0954       | 0.032*     |
| C16  | 0.35748 (14) | 0.92782 (15) | -0.07856 (10) | 0.0246 (4) |
| H16  | 0.2864       | 0.9711       | -0.0572       | 0.029*     |
| C17  | 0.49498 (16) | 0.80561 (16) | -0.18567 (11) | 0.0298 (5) |
| H17A | 0.4440       | 0.8117       | -0.2135       | 0.036*     |
| H17B | 0.5654       | 0.7628       | -0.2068       | 0.036*     |
| C18  | 0.43936 (13) | 0.91824 (14) | -0.03720 (10) | 0.0199 (4) |
| H18A | 0.4441       | 0.9879       | -0.0432       | 0.024*     |
| H18B | 0.4165       | 0.8870       | 0.0167        | 0.024*     |
| C19  | 0.39209 (15) | 0.97930 (15) | -0.16090 (11) | 0.0276 (4) |
| H19A | 0.3957       | 1.0492       | -0.1666       | 0.033*     |
| H19B | 0.3396       | 0.9868       | -0.1881       | 0.033*     |
| C20  | 0.50118 (15) | 0.91321 (16) | -0.19370 (10) | 0.0262 (4) |
| H20  | 0.5238       | 0.9472       | -0.2477       | 0.031*     |
| C21  | 0.58291 (14) | 0.90275 (15) | -0.15148 (10) | 0.0215 (4) |
| H21A | 0.6538       | 0.8611       | -0.1730       | 0.026*     |
| H21B | 0.5876       | 0.9721       | -0.1568       | 0.026*     |
| C22  | 0.37224 (13) | 0.76579 (13) | 0.15094 (9)   | 0.0175 (4) |
| C23  | 0.26509 (14) | 0.82850 (14) | 0.17133 (11)  | 0.0239 (4) |
| H23  | 0.2530       | 0.8945       | 0.1784        | 0.029*     |
| C24  | 0.18098 (14) | 0.79536 (14) | 0.18072 (11)  | 0.0244 (4) |
| H24  | 0.1113       | 0.8384       | 0.1948        | 0.029*     |
| C25  | 0.19442 (14) | 0.69776 (14) | 0.17003 (10)  | 0.0207 (4) |
| C26  | 0.10572 (14) | 0.66529 (15) | 0.17852 (10)  | 0.0230 (4) |
| H26  | 0.0363       | 0.7089       | 0.1924        | 0.028*     |
| C27  | 0.11792 (15) | 0.57242 (15) | 0.16719 (10)  | 0.0257 (4) |
| H27  | 0.0576       | 0.5514       | 0.1735        | 0.031*     |
| C28  | 0.22060 (15) | 0.50839 (15) | 0.14610 (10)  | 0.0243 (4) |
| H28  | 0.2296       | 0.4440       | 0.1377        | 0.029*     |
| C29  | 0.30838 (14) | 0.53796 (14) | 0.13740 (10)  | 0.0209 (4) |
| H29  | 0.3770       | 0.4938       | 0.1224        | 0.025*     |
| C30  | 0.29912 (13) | 0.63255 (13) | 0.15019 (9)   | 0.0178 (4) |
| C31  | 0.38928 (13) | 0.66629 (13) | 0.14309 (9)   | 0.0171 (3) |
| C32  | 0.49285 (13) | 0.59156 (13) | 0.13748 (9)   | 0.0161 (3) |
| H32  | 0.4946       | 0.5213       | 0.1482        | 0.019*     |
| C33  | 0.68321 (13) | 0.52224 (13) | 0.12298 (9)   | 0.0154 (3) |
| C34  | 0.76264 (13) | 0.54495 (14) | 0.04841 (9)   | 0.0189 (4) |
| H34A | 0.7351       | 0.5455       | 0.0075        | 0.023*     |
| H34B | 0.7713       | 0.6141       | 0.0386        | 0.023*     |
| C35  | 0.87028 (14) | 0.46254 (14) | 0.05038 (10)  | 0.0232 (4) |
| H35  | 0.9212       | 0.4782       | 0.0015        | 0.028*     |
| C36  | 0.91327 (14) | 0.46301 (15) | 0.11315 (10)  | 0.0231 (4) |
| H36A | 0.9832       | 0.4105       | 0.1144        | 0.028*     |
| H36B | 0.9225       | 0.5317       | 0.1041        | 0.028*     |

|      |               |               |               |             |
|------|---------------|---------------|---------------|-------------|
| C37  | 0.83511 (14)  | 0.43872 (14)  | 0.18776 (10)  | 0.0220 (4)  |
| H37  | 0.8632        | 0.4387        | 0.2288        | 0.026*      |
| C38  | 0.72696 (13)  | 0.52142 (13)  | 0.18607 (10)  | 0.0182 (4)  |
| H38A | 0.6766        | 0.5062        | 0.2345        | 0.022*      |
| H38B | 0.7351        | 0.5904        | 0.1779        | 0.022*      |
| C39  | 0.85710 (15)  | 0.35565 (15)  | 0.06471 (11)  | 0.0285 (4)  |
| H39A | 0.8307        | 0.3543        | 0.0239        | 0.034*      |
| H39B | 0.9265        | 0.3022        | 0.0661        | 0.034*      |
| C40  | 0.82098 (15)  | 0.33239 (14)  | 0.20207 (11)  | 0.0269 (4)  |
| H40A | 0.7706        | 0.3168        | 0.2504        | 0.032*      |
| H40B | 0.8899        | 0.2784        | 0.2044        | 0.032*      |
| C41  | 0.77850 (15)  | 0.33235 (14)  | 0.13903 (12)  | 0.0264 (4)  |
| H41A | 0.7695        | 0.2628        | 0.1482        | 0.032*      |
| C42  | 0.67056 (14)  | 0.41526 (13)  | 0.13678 (11)  | 0.0225 (4)  |
| H42A | 0.6424        | 0.4149        | 0.0965        | 0.027*      |
| H42B | 0.6195        | 0.3995        | 0.1847        | 0.027*      |
| Co2  | 0.886744 (17) | 0.185711 (17) | 0.585004 (12) | 0.01390 (6) |
| O3   | 1.00067 (9)   | 0.10345 (9)   | 0.63422 (6)   | 0.0172 (2)  |
| O4   | 0.76314 (9)   | 0.13745 (9)   | 0.62356 (6)   | 0.0182 (3)  |
| N3   | 0.87112 (10)  | 0.31587 (10)  | 0.60847 (7)   | 0.0139 (3)  |
| N4   | 0.90708 (11)  | 0.17854 (10)  | 0.48169 (8)   | 0.0143 (3)  |
| C43  | 1.06441 (13)  | 0.14134 (13)  | 0.64622 (9)   | 0.0149 (3)  |
| C44  | 1.16275 (13)  | 0.06899 (13)  | 0.66230 (9)   | 0.0183 (4)  |
| H44  | 1.1779        | -0.0011       | 0.6623        | 0.022*      |
| C45  | 1.23434 (13)  | 0.09768 (13)  | 0.67740 (9)   | 0.0187 (4)  |
| H45  | 1.2983        | 0.0472        | 0.6881        | 0.022*      |
| C46  | 1.21613 (13)  | 0.20208 (13)  | 0.67764 (9)   | 0.0158 (3)  |
| C47  | 1.29146 (13)  | 0.23070 (14)  | 0.69404 (9)   | 0.0191 (4)  |
| H47  | 1.3538        | 0.1791        | 0.7067        | 0.023*      |
| C48  | 1.27664 (14)  | 0.33105 (14)  | 0.69216 (10)  | 0.0214 (4)  |
| H48  | 1.3280        | 0.3493        | 0.7033        | 0.026*      |
| C49  | 1.18440 (14)  | 0.40625 (14)  | 0.67358 (10)  | 0.0220 (4)  |
| H49  | 1.1737        | 0.4763        | 0.6717        | 0.026*      |
| C50  | 1.10900 (14)  | 0.38079 (14)  | 0.65797 (10)  | 0.0200 (4)  |
| H50  | 1.0473        | 0.4338        | 0.6455        | 0.024*      |
| C51  | 1.12092 (13)  | 0.27747 (13)  | 0.66006 (9)   | 0.0158 (3)  |
| C52  | 1.04294 (13)  | 0.24605 (13)  | 0.64497 (9)   | 0.0153 (3)  |
| C53  | 0.94385 (13)  | 0.32323 (13)  | 0.63285 (9)   | 0.0153 (3)  |
| H53  | 0.9304        | 0.3868        | 0.6441        | 0.018*      |
| C54  | 0.77189 (13)  | 0.40338 (12)  | 0.60191 (9)   | 0.0143 (3)  |
| C55  | 0.77324 (13)  | 0.50404 (13)  | 0.61211 (10)  | 0.0176 (4)  |
| H55A | 0.8321        | 0.5282        | 0.5744        | 0.021*      |
| H55B | 0.7850        | 0.4913        | 0.6622        | 0.021*      |
| C56  | 0.66674 (14)  | 0.58790 (13)  | 0.60358 (10)  | 0.0198 (4)  |
| H56  | 0.6685        | 0.6532        | 0.6102        | 0.024*      |
| C57  | 0.64941 (15)  | 0.60857 (14)  | 0.52579 (11)  | 0.0241 (4)  |
| H57A | 0.7076        | 0.6330        | 0.4873        | 0.029*      |
| H57B | 0.5817        | 0.6630        | 0.5199        | 0.029*      |
| C58  | 0.64665 (14)  | 0.50811 (14)  | 0.51598 (10)  | 0.0218 (4)  |

## supplementary materials

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|      |              |              |              |            |
|------|--------------|--------------|--------------|------------|
| H58  | 0.6350       | 0.5210       | 0.4653       | 0.026*     |
| C59  | 0.75287 (13) | 0.42466 (13) | 0.52432 (9)  | 0.0177 (4) |
| H59A | 0.7520       | 0.3600       | 0.5171       | 0.021*     |
| H59B | 0.8114       | 0.4482       | 0.4856       | 0.021*     |
| C60  | 0.57627 (14) | 0.55089 (14) | 0.66338 (10) | 0.0216 (4) |
| H60A | 0.5871       | 0.5387       | 0.7136       | 0.026*     |
| H60B | 0.5077       | 0.6046       | 0.6586       | 0.026*     |
| C61  | 0.57431 (14) | 0.45053 (14) | 0.65338 (10) | 0.0208 (4) |
| H61  | 0.5153       | 0.4261       | 0.6922       | 0.025*     |
| C62  | 0.55641 (14) | 0.47087 (14) | 0.57561 (11) | 0.0230 (4) |
| H62A | 0.5539       | 0.4065       | 0.5690       | 0.028*     |
| H62B | 0.4878       | 0.5241       | 0.5703       | 0.028*     |
| C63  | 0.68031 (13) | 0.36759 (13) | 0.66175 (9)  | 0.0171 (3) |
| H63A | 0.6786       | 0.3020       | 0.6566       | 0.020*     |
| H63B | 0.6917       | 0.3546       | 0.7119       | 0.020*     |
| C64  | 0.70488 (13) | 0.13519 (12) | 0.58424 (10) | 0.0175 (4) |
| C65  | 0.60514 (14) | 0.11461 (14) | 0.62443 (11) | 0.0233 (4) |
| H65  | 0.5848       | 0.1052       | 0.6770       | 0.028*     |
| C66  | 0.53954 (14) | 0.10844 (14) | 0.58876 (12) | 0.0261 (4) |
| H66  | 0.4754       | 0.0923       | 0.6173       | 0.031*     |
| C67  | 0.56351 (14) | 0.12523 (13) | 0.51025 (11) | 0.0221 (4) |
| C68  | 0.49154 (15) | 0.12397 (14) | 0.47355 (13) | 0.0288 (5) |
| H68  | 0.4273       | 0.1084       | 0.5025       | 0.035*     |
| C69  | 0.51192 (16) | 0.14445 (15) | 0.39802 (13) | 0.0318 (5) |
| H69  | 0.4632       | 0.1422       | 0.3744       | 0.038*     |
| C70  | 0.60583 (17) | 0.16889 (15) | 0.35577 (12) | 0.0311 (5) |
| H70  | 0.6201       | 0.1847       | 0.3029       | 0.037*     |
| C71  | 0.67797 (15) | 0.17039 (14) | 0.38951 (11) | 0.0246 (4) |
| H71  | 0.7411       | 0.1872       | 0.3593       | 0.029*     |
| C72  | 0.66044 (14) | 0.14760 (13) | 0.46771 (10) | 0.0190 (4) |
| C73  | 0.73407 (13) | 0.14876 (12) | 0.50606 (10) | 0.0165 (3) |
| C74  | 0.83515 (13) | 0.16210 (12) | 0.46196 (9)  | 0.0158 (3) |
| H74  | 0.8516       | 0.1584       | 0.4118       | 0.019*     |
| C75  | 1.00216 (13) | 0.19701 (13) | 0.42137 (9)  | 0.0142 (3) |
| C76  | 0.96679 (13) | 0.29700 (13) | 0.36171 (9)  | 0.0169 (3) |
| H76A | 0.9173       | 0.2890       | 0.3388       | 0.020*     |
| H76B | 0.9290       | 0.3555       | 0.3853       | 0.020*     |
| C77  | 1.06352 (14) | 0.32036 (13) | 0.30118 (10) | 0.0192 (4) |
| H77  | 1.0397       | 0.3849       | 0.2624       | 0.023*     |
| C78  | 1.13780 (14) | 0.33519 (14) | 0.33722 (10) | 0.0213 (4) |
| H78A | 1.1002       | 0.3939       | 0.3606       | 0.026*     |
| H78B | 1.2000       | 0.3514       | 0.2986       | 0.026*     |
| C79  | 1.17465 (14) | 0.23610 (14) | 0.39641 (10) | 0.0208 (4) |
| H79  | 1.2231       | 0.2458       | 0.4199       | 0.025*     |
| C80  | 1.07802 (13) | 0.21172 (14) | 0.45621 (10) | 0.0184 (4) |
| H80A | 1.1018       | 0.1479       | 0.4946       | 0.022*     |
| H80B | 1.0404       | 0.2691       | 0.4808       | 0.022*     |
| C81  | 1.23330 (14) | 0.14586 (14) | 0.35980 (11) | 0.0239 (4) |
| H81A | 1.2581       | 0.0818       | 0.3977       | 0.029*     |



|      |              |              |              |            |
|------|--------------|--------------|--------------|------------|
| H81B | 1.2961       | 0.1606       | 0.3212       | 0.029*     |
| C82  | 1.15870 (14) | 0.13049 (14) | 0.32418 (10) | 0.0220 (4) |
| H82  | 1.1972       | 0.0716       | 0.3003       | 0.026*     |
| C83  | 1.12133 (14) | 0.22924 (14) | 0.26513 (10) | 0.0222 (4) |
| H83A | 1.0729       | 0.2195       | 0.2422       | 0.027*     |
| H83B | 1.1831       | 0.2441       | 0.2254       | 0.027*     |
| C84  | 1.06196 (13) | 0.10605 (13) | 0.38499 (10) | 0.0188 (4) |
| H84A | 1.0141       | 0.0946       | 0.3626       | 0.023*     |
| H84B | 1.0858       | 0.0421       | 0.4233       | 0.023*     |

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

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Co1 | 0.01407 (12) | 0.01428 (12) | 0.01469 (12) | -0.00514 (9) | -0.00332 (9) | -0.00202 (9) |
| O2  | 0.0169 (6)   | 0.0188 (6)   | 0.0221 (6)   | -0.0056 (5)  | -0.0016 (5)  | -0.0049 (5)  |
| O1  | 0.0197 (6)   | 0.0236 (7)   | 0.0159 (6)   | -0.0113 (5)  | -0.0040 (5)  | -0.0015 (5)  |
| N1  | 0.0145 (7)   | 0.0129 (7)   | 0.0154 (7)   | -0.0026 (5)  | -0.0047 (6)  | -0.0039 (6)  |
| N2  | 0.0136 (7)   | 0.0157 (7)   | 0.0139 (7)   | -0.0037 (6)  | -0.0023 (5)  | -0.0035 (6)  |
| C1  | 0.0155 (8)   | 0.0152 (8)   | 0.0189 (9)   | -0.0049 (7)  | -0.0038 (7)  | -0.0039 (7)  |
| C2  | 0.0212 (9)   | 0.0211 (9)   | 0.0170 (9)   | -0.0057 (7)  | -0.0075 (7)  | -0.0016 (7)  |
| C3  | 0.0177 (9)   | 0.0190 (9)   | 0.0252 (9)   | -0.0053 (7)  | -0.0103 (7)  | -0.0045 (7)  |
| C4  | 0.0162 (8)   | 0.0127 (8)   | 0.0225 (9)   | -0.0028 (7)  | -0.0052 (7)  | -0.0048 (7)  |
| C5  | 0.0167 (9)   | 0.0176 (9)   | 0.0287 (10)  | -0.0047 (7)  | -0.0073 (7)  | -0.0060 (8)  |
| C6  | 0.0149 (9)   | 0.0194 (9)   | 0.0297 (10)  | -0.0066 (7)  | -0.0007 (7)  | -0.0053 (8)  |
| C7  | 0.0203 (9)   | 0.0163 (9)   | 0.0209 (9)   | -0.0044 (7)  | -0.0014 (7)  | -0.0048 (7)  |
| C8  | 0.0167 (8)   | 0.0141 (8)   | 0.0217 (9)   | -0.0027 (7)  | -0.0050 (7)  | -0.0059 (7)  |
| C9  | 0.0157 (8)   | 0.0092 (8)   | 0.0196 (9)   | -0.0020 (6)  | -0.0035 (7)  | -0.0039 (7)  |
| C10 | 0.0140 (8)   | 0.0130 (8)   | 0.0188 (9)   | -0.0038 (6)  | -0.0040 (7)  | -0.0049 (7)  |
| C11 | 0.0171 (8)   | 0.0126 (8)   | 0.0142 (8)   | -0.0039 (7)  | -0.0035 (7)  | -0.0029 (6)  |
| C12 | 0.0155 (8)   | 0.0185 (9)   | 0.0153 (8)   | -0.0061 (7)  | -0.0048 (7)  | -0.0049 (7)  |
| C13 | 0.0206 (9)   | 0.0191 (9)   | 0.0239 (9)   | -0.0061 (7)  | -0.0080 (7)  | -0.0065 (7)  |
| C14 | 0.0279 (10)  | 0.0247 (10)  | 0.0294 (10)  | -0.0114 (8)  | -0.0112 (8)  | -0.0083 (8)  |
| C15 | 0.0231 (10)  | 0.0374 (11)  | 0.0261 (10)  | -0.0141 (9)  | -0.0117 (8)  | -0.0036 (9)  |
| C16 | 0.0176 (9)   | 0.0303 (10)  | 0.0261 (10)  | -0.0027 (8)  | -0.0090 (8)  | -0.0083 (8)  |
| C17 | 0.0322 (11)  | 0.0407 (12)  | 0.0248 (10)  | -0.0101 (9)  | -0.0107 (9)  | -0.0146 (9)  |
| C18 | 0.0188 (9)   | 0.0209 (9)   | 0.0205 (9)   | -0.0028 (7)  | -0.0072 (7)  | -0.0065 (7)  |
| C19 | 0.0290 (11)  | 0.0281 (10)  | 0.0280 (10)  | -0.0064 (8)  | -0.0170 (9)  | -0.0020 (8)  |
| C20 | 0.0282 (10)  | 0.0362 (11)  | 0.0167 (9)   | -0.0130 (9)  | -0.0084 (8)  | -0.0027 (8)  |
| C21 | 0.0219 (9)   | 0.0270 (10)  | 0.0174 (9)   | -0.0101 (8)  | -0.0059 (7)  | -0.0032 (8)  |
| C22 | 0.0168 (8)   | 0.0173 (9)   | 0.0144 (8)   | -0.0049 (7)  | -0.0022 (7)  | -0.0005 (7)  |
| C23 | 0.0202 (9)   | 0.0164 (9)   | 0.0284 (10)  | -0.0019 (7)  | -0.0036 (8)  | -0.0030 (8)  |
| C24 | 0.0150 (9)   | 0.0210 (9)   | 0.0266 (10)  | 0.0005 (7)   | -0.0027 (7)  | -0.0013 (8)  |
| C25 | 0.0171 (9)   | 0.0230 (9)   | 0.0163 (9)   | -0.0047 (7)  | -0.0045 (7)  | 0.0015 (7)   |
| C26 | 0.0134 (8)   | 0.0286 (10)  | 0.0195 (9)   | -0.0051 (7)  | -0.0050 (7)  | 0.0030 (8)   |
| C27 | 0.0202 (9)   | 0.0336 (11)  | 0.0231 (10)  | -0.0138 (8)  | -0.0078 (8)  | 0.0021 (8)   |
| C28 | 0.0250 (10)  | 0.0288 (10)  | 0.0225 (10)  | -0.0128 (8)  | -0.0069 (8)  | -0.0038 (8)  |
| C29 | 0.0174 (9)   | 0.0255 (10)  | 0.0188 (9)   | -0.0060 (7)  | -0.0033 (7)  | -0.0054 (8)  |
| C30 | 0.0159 (8)   | 0.0197 (9)   | 0.0133 (8)   | -0.0052 (7)  | -0.0035 (7)  | 0.0015 (7)   |

## supplementary materials

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|     |              |              |              |              |              |              |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| C31 | 0.0154 (8)   | 0.0188 (9)   | 0.0144 (8)   | -0.0055 (7)  | -0.0021 (7)  | -0.0015 (7)  |
| C32 | 0.0177 (8)   | 0.0162 (8)   | 0.0140 (8)   | -0.0061 (7)  | -0.0031 (7)  | -0.0026 (7)  |
| C33 | 0.0133 (8)   | 0.0155 (8)   | 0.0173 (8)   | -0.0031 (7)  | -0.0041 (7)  | -0.0045 (7)  |
| C34 | 0.0168 (9)   | 0.0221 (9)   | 0.0158 (9)   | -0.0056 (7)  | -0.0020 (7)  | -0.0041 (7)  |
| C35 | 0.0159 (9)   | 0.0270 (10)  | 0.0217 (9)   | -0.0012 (7)  | -0.0008 (7)  | -0.0087 (8)  |
| C36 | 0.0147 (9)   | 0.0229 (10)  | 0.0304 (10)  | -0.0026 (7)  | -0.0058 (8)  | -0.0073 (8)  |
| C37 | 0.0190 (9)   | 0.0237 (9)   | 0.0223 (9)   | -0.0017 (7)  | -0.0094 (7)  | -0.0050 (8)  |
| C38 | 0.0183 (9)   | 0.0175 (9)   | 0.0158 (8)   | -0.0028 (7)  | -0.0035 (7)  | -0.0035 (7)  |
| C39 | 0.0215 (10)  | 0.0285 (11)  | 0.0360 (11)  | 0.0034 (8)   | -0.0083 (8)  | -0.0186 (9)  |
| C40 | 0.0205 (10)  | 0.0210 (10)  | 0.0304 (11)  | -0.0006 (8)  | -0.0071 (8)  | -0.0005 (8)  |
| C41 | 0.0215 (10)  | 0.0144 (9)   | 0.0433 (12)  | -0.0022 (7)  | -0.0090 (9)  | -0.0089 (8)  |
| C42 | 0.0165 (9)   | 0.0170 (9)   | 0.0343 (11)  | -0.0041 (7)  | -0.0063 (8)  | -0.0070 (8)  |
| Co2 | 0.01420 (12) | 0.01327 (11) | 0.01472 (12) | -0.00393 (9) | -0.00410 (9) | -0.00341 (9) |
| O3  | 0.0180 (6)   | 0.0151 (6)   | 0.0198 (6)   | -0.0049 (5)  | -0.0071 (5)  | -0.0031 (5)  |
| O4  | 0.0189 (6)   | 0.0195 (6)   | 0.0180 (6)   | -0.0086 (5)  | -0.0022 (5)  | -0.0053 (5)  |
| N3  | 0.0130 (7)   | 0.0136 (7)   | 0.0137 (7)   | -0.0028 (5)  | -0.0031 (5)  | -0.0029 (5)  |
| N4  | 0.0152 (7)   | 0.0113 (7)   | 0.0157 (7)   | -0.0040 (5)  | -0.0037 (6)  | -0.0020 (5)  |
| C43 | 0.0161 (8)   | 0.0180 (8)   | 0.0097 (8)   | -0.0059 (7)  | -0.0025 (6)  | -0.0016 (6)  |
| C44 | 0.0190 (9)   | 0.0149 (8)   | 0.0176 (9)   | -0.0025 (7)  | -0.0040 (7)  | -0.0028 (7)  |
| C45 | 0.0144 (8)   | 0.0188 (9)   | 0.0175 (9)   | -0.0007 (7)  | -0.0041 (7)  | -0.0021 (7)  |
| C46 | 0.0143 (8)   | 0.0193 (9)   | 0.0117 (8)   | -0.0047 (7)  | -0.0016 (6)  | -0.0027 (7)  |
| C47 | 0.0126 (8)   | 0.0260 (10)  | 0.0165 (9)   | -0.0022 (7)  | -0.0030 (7)  | -0.0068 (7)  |
| C48 | 0.0185 (9)   | 0.0289 (10)  | 0.0208 (9)   | -0.0090 (8)  | -0.0055 (7)  | -0.0077 (8)  |
| C49 | 0.0225 (9)   | 0.0207 (9)   | 0.0269 (10)  | -0.0067 (8)  | -0.0058 (8)  | -0.0102 (8)  |
| C50 | 0.0165 (9)   | 0.0201 (9)   | 0.0232 (9)   | -0.0012 (7)  | -0.0063 (7)  | -0.0080 (7)  |
| C51 | 0.0151 (8)   | 0.0198 (9)   | 0.0125 (8)   | -0.0048 (7)  | -0.0025 (6)  | -0.0051 (7)  |
| C52 | 0.0137 (8)   | 0.0158 (8)   | 0.0143 (8)   | -0.0029 (7)  | -0.0031 (6)  | -0.0026 (7)  |
| C53 | 0.0162 (8)   | 0.0149 (8)   | 0.0145 (8)   | -0.0045 (7)  | -0.0022 (6)  | -0.0047 (7)  |
| C54 | 0.0126 (8)   | 0.0134 (8)   | 0.0165 (8)   | -0.0006 (6)  | -0.0054 (6)  | -0.0048 (7)  |
| C55 | 0.0153 (8)   | 0.0161 (8)   | 0.0234 (9)   | -0.0036 (7)  | -0.0061 (7)  | -0.0067 (7)  |
| C56 | 0.0177 (9)   | 0.0149 (9)   | 0.0280 (10)  | -0.0018 (7)  | -0.0077 (7)  | -0.0075 (7)  |
| C57 | 0.0231 (10)  | 0.0163 (9)   | 0.0281 (10)  | 0.0011 (7)   | -0.0107 (8)  | -0.0028 (8)  |
| C58 | 0.0221 (9)   | 0.0209 (9)   | 0.0211 (9)   | 0.0007 (7)   | -0.0118 (8)  | -0.0051 (7)  |
| C59 | 0.0187 (9)   | 0.0177 (9)   | 0.0170 (8)   | -0.0029 (7)  | -0.0063 (7)  | -0.0051 (7)  |
| C60 | 0.0167 (9)   | 0.0196 (9)   | 0.0270 (10)  | 0.0014 (7)   | -0.0061 (7)  | -0.0104 (8)  |
| C61 | 0.0146 (8)   | 0.0211 (9)   | 0.0259 (10)  | -0.0040 (7)  | -0.0021 (7)  | -0.0085 (8)  |
| C62 | 0.0156 (9)   | 0.0231 (10)  | 0.0343 (11)  | -0.0005 (7)  | -0.0122 (8)  | -0.0114 (8)  |
| C63 | 0.0156 (8)   | 0.0166 (8)   | 0.0182 (9)   | -0.0029 (7)  | -0.0029 (7)  | -0.0064 (7)  |
| C64 | 0.0159 (8)   | 0.0107 (8)   | 0.0258 (9)   | -0.0031 (7)  | -0.0038 (7)  | -0.0061 (7)  |
| C65 | 0.0195 (9)   | 0.0232 (10)  | 0.0275 (10)  | -0.0086 (8)  | 0.0023 (8)   | -0.0114 (8)  |
| C66 | 0.0142 (9)   | 0.0229 (10)  | 0.0422 (12)  | -0.0073 (7)  | 0.0022 (8)   | -0.0151 (9)  |
| C67 | 0.0162 (9)   | 0.0146 (9)   | 0.0381 (11)  | -0.0023 (7)  | -0.0078 (8)  | -0.0105 (8)  |
| C68 | 0.0166 (9)   | 0.0195 (10)  | 0.0558 (14)  | -0.0020 (8)  | -0.0125 (9)  | -0.0155 (9)  |
| C69 | 0.0283 (11)  | 0.0212 (10)  | 0.0568 (14)  | -0.0014 (8)  | -0.0279 (10) | -0.0124 (10) |
| C70 | 0.0367 (12)  | 0.0248 (10)  | 0.0373 (12)  | -0.0044 (9)  | -0.0233 (10) | -0.0055 (9)  |
| C71 | 0.0263 (10)  | 0.0191 (9)   | 0.0317 (11)  | -0.0058 (8)  | -0.0139 (8)  | -0.0043 (8)  |
| C72 | 0.0185 (9)   | 0.0111 (8)   | 0.0286 (10)  | -0.0017 (7)  | -0.0089 (7)  | -0.0060 (7)  |
| C73 | 0.0157 (8)   | 0.0114 (8)   | 0.0232 (9)   | -0.0040 (7)  | -0.0059 (7)  | -0.0039 (7)  |
| C74 | 0.0188 (8)   | 0.0124 (8)   | 0.0155 (8)   | -0.0032 (7)  | -0.0053 (7)  | -0.0027 (7)  |

|     |            |             |             |             |             |             |
|-----|------------|-------------|-------------|-------------|-------------|-------------|
| C75 | 0.0140 (8) | 0.0143 (8)  | 0.0141 (8)  | -0.0046 (6) | -0.0019 (6) | -0.0040 (6) |
| C76 | 0.0169 (8) | 0.0141 (8)  | 0.0190 (9)  | -0.0027 (7) | -0.0062 (7) | -0.0033 (7) |
| C77 | 0.0222 (9) | 0.0160 (9)  | 0.0169 (9)  | -0.0071 (7) | -0.0038 (7) | 0.0001 (7)  |
| C78 | 0.0221 (9) | 0.0197 (9)  | 0.0231 (9)  | -0.0119 (8) | 0.0011 (7)  | -0.0062 (7) |
| C79 | 0.0175 (9) | 0.0255 (10) | 0.0211 (9)  | -0.0104 (7) | -0.0037 (7) | -0.0042 (8) |
| C80 | 0.0171 (9) | 0.0202 (9)  | 0.0181 (9)  | -0.0068 (7) | -0.0042 (7) | -0.0034 (7) |
| C81 | 0.0169 (9) | 0.0223 (10) | 0.0251 (10) | -0.0050 (7) | -0.0002 (7) | -0.0020 (8) |
| C82 | 0.0200 (9) | 0.0186 (9)  | 0.0245 (10) | -0.0047 (7) | 0.0027 (7)  | -0.0101 (8) |
| C83 | 0.0214 (9) | 0.0283 (10) | 0.0173 (9)  | -0.0100 (8) | 0.0020 (7)  | -0.0091 (8) |
| C84 | 0.0175 (9) | 0.0153 (8)  | 0.0231 (9)  | -0.0049 (7) | -0.0018 (7) | -0.0066 (7) |

*Geometric parameters (Å, °)*

|          |             |          |             |
|----------|-------------|----------|-------------|
| Co1—O1   | 1.9051 (12) | Co2—O3   | 1.9139 (12) |
| Co1—O2   | 1.9192 (12) | Co2—O4   | 1.9194 (12) |
| Co1—N1   | 1.9962 (14) | Co2—N3   | 1.9945 (13) |
| Co1—N2   | 2.0019 (14) | Co2—N4   | 1.9849 (14) |
| O2—C22   | 1.306 (2)   | O3—C43   | 1.3088 (19) |
| O1—C1    | 1.303 (2)   | O4—C64   | 1.300 (2)   |
| N1—C11   | 1.295 (2)   | N3—C53   | 1.299 (2)   |
| N1—C12   | 1.497 (2)   | N3—C54   | 1.493 (2)   |
| N2—C32   | 1.295 (2)   | N4—C74   | 1.300 (2)   |
| N2—C33   | 1.491 (2)   | N4—C75   | 1.500 (2)   |
| C1—C10   | 1.416 (2)   | C43—C52  | 1.414 (2)   |
| C1—C2    | 1.438 (2)   | C43—C44  | 1.435 (2)   |
| C2—C3    | 1.352 (2)   | C44—C45  | 1.350 (2)   |
| C2—H2    | 0.9500      | C44—H44  | 0.9500      |
| C3—C4    | 1.426 (2)   | C45—C46  | 1.427 (2)   |
| C3—H3    | 0.9500      | C45—H45  | 0.9500      |
| C4—C5    | 1.411 (2)   | C46—C47  | 1.412 (2)   |
| C4—C9    | 1.425 (2)   | C46—C51  | 1.425 (2)   |
| C5—C6    | 1.368 (3)   | C47—C48  | 1.368 (3)   |
| C5—H5    | 0.9500      | C47—H47  | 0.9500      |
| C6—C7    | 1.404 (2)   | C48—C49  | 1.399 (3)   |
| C6—H6    | 0.9500      | C48—H48  | 0.9500      |
| C7—C8    | 1.375 (2)   | C49—C50  | 1.375 (2)   |
| C7—H7    | 0.9500      | C49—H49  | 0.9500      |
| C8—C9    | 1.418 (2)   | C50—C51  | 1.418 (2)   |
| C8—H8    | 0.9500      | C50—H50  | 0.9500      |
| C9—C10   | 1.458 (2)   | C51—C52  | 1.457 (2)   |
| C10—C11  | 1.442 (2)   | C52—C53  | 1.447 (2)   |
| C11—H11  | 0.9500      | C53—H53  | 0.9500      |
| C12—C21  | 1.532 (2)   | C54—C55  | 1.533 (2)   |
| C12—C13  | 1.534 (2)   | C54—C59  | 1.534 (2)   |
| C12—C18  | 1.540 (2)   | C54—C63  | 1.538 (2)   |
| C13—C14  | 1.531 (2)   | C55—C56  | 1.544 (2)   |
| C13—H13A | 0.9900      | C55—H55A | 0.9900      |
| C13—H13B | 0.9900      | C55—H55B | 0.9900      |
| C14—C17  | 1.527 (3)   | C56—C57  | 1.530 (3)   |

## supplementary materials

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|          |           |          |           |
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| C14—C15  | 1.529 (3) | C56—C60  | 1.534 (3) |
| C14—H14  | 1.0000    | C56—H56  | 1.0000    |
| C15—C16  | 1.536 (3) | C57—C58  | 1.534 (2) |
| C15—H15A | 0.9900    | C57—H57A | 0.9900    |
| C15—H15B | 0.9900    | C57—H57B | 0.9900    |
| C16—C19  | 1.524 (3) | C58—C62  | 1.531 (3) |
| C16—C18  | 1.541 (2) | C58—C59  | 1.538 (2) |
| C16—H16  | 1.0000    | C58—H58  | 1.0000    |
| C17—C20  | 1.530 (3) | C59—H59A | 0.9900    |
| C17—H17A | 0.9900    | C59—H59B | 0.9900    |
| C17—H17B | 0.9900    | C60—C61  | 1.530 (2) |
| C18—H18A | 0.9900    | C60—H60A | 0.9900    |
| C18—H18B | 0.9900    | C60—H60B | 0.9900    |
| C19—C20  | 1.533 (3) | C61—C63  | 1.533 (2) |
| C19—H19A | 0.9900    | C61—C62  | 1.534 (3) |
| C19—H19B | 0.9900    | C61—H61  | 1.0000    |
| C20—C21  | 1.547 (2) | C62—H62A | 0.9900    |
| C20—H20  | 1.0000    | C62—H62B | 0.9900    |
| C21—H21A | 0.9900    | C63—H63A | 0.9900    |
| C21—H21B | 0.9900    | C63—H63B | 0.9900    |
| C22—C31  | 1.414 (2) | C64—C73  | 1.415 (2) |
| C22—C23  | 1.439 (2) | C64—C65  | 1.438 (2) |
| C23—C24  | 1.356 (3) | C65—C66  | 1.357 (3) |
| C23—H23  | 0.9500    | C65—H65  | 0.9500    |
| C24—C25  | 1.424 (3) | C66—C67  | 1.418 (3) |
| C24—H24  | 0.9500    | C66—H66  | 0.9500    |
| C25—C26  | 1.415 (2) | C67—C68  | 1.416 (2) |
| C25—C30  | 1.426 (2) | C67—C72  | 1.423 (2) |
| C26—C27  | 1.367 (3) | C68—C69  | 1.360 (3) |
| C26—H26  | 0.9500    | C68—H68  | 0.9500    |
| C27—C28  | 1.404 (3) | C69—C70  | 1.398 (3) |
| C27—H27  | 0.9500    | C69—H69  | 0.9500    |
| C28—C29  | 1.377 (2) | C70—C71  | 1.377 (3) |
| C28—H28  | 0.9500    | C70—H70  | 0.9500    |
| C29—C30  | 1.417 (2) | C71—C72  | 1.410 (3) |
| C29—H29  | 0.9500    | C71—H71  | 0.9500    |
| C30—C31  | 1.454 (2) | C72—C73  | 1.459 (2) |
| C31—C32  | 1.443 (2) | C73—C74  | 1.436 (2) |
| C32—H32  | 0.9500    | C74—H74  | 0.9500    |
| C33—C42  | 1.532 (2) | C75—C80  | 1.533 (2) |
| C33—C34  | 1.536 (2) | C75—C84  | 1.538 (2) |
| C33—C38  | 1.538 (2) | C75—C76  | 1.539 (2) |
| C34—C35  | 1.532 (2) | C76—C77  | 1.536 (2) |
| C34—H34A | 0.9900    | C76—H76A | 0.9900    |
| C34—H34B | 0.9900    | C76—H76B | 0.9900    |
| C35—C39  | 1.532 (3) | C77—C78  | 1.531 (2) |
| C35—C36  | 1.533 (3) | C77—C83  | 1.534 (2) |
| C35—H35  | 1.0000    | C77—H77  | 1.0000    |
| C36—C37  | 1.531 (3) | C78—C79  | 1.532 (3) |

|            |             |             |             |
|------------|-------------|-------------|-------------|
| C36—H36A   | 0.9900      | C78—H78A    | 0.9900      |
| C36—H36B   | 0.9900      | C78—H78B    | 0.9900      |
| C37—C40    | 1.529 (3)   | C79—C81     | 1.531 (3)   |
| C37—C38    | 1.539 (2)   | C79—C80     | 1.533 (2)   |
| C37—H37    | 1.0000      | C79—H79     | 1.0000      |
| C38—H38A   | 0.9900      | C80—H80A    | 0.9900      |
| C38—H38B   | 0.9900      | C80—H80B    | 0.9900      |
| C39—C41    | 1.528 (3)   | C81—C82     | 1.533 (3)   |
| C39—H39A   | 0.9900      | C81—H81A    | 0.9900      |
| C39—H39B   | 0.9900      | C81—H81B    | 0.9900      |
| C40—C41    | 1.531 (3)   | C82—C83     | 1.530 (3)   |
| C40—H40A   | 0.9900      | C82—C84     | 1.543 (2)   |
| C40—H40B   | 0.9900      | C82—H82     | 1.0000      |
| C41—C42    | 1.539 (2)   | C83—H83A    | 0.9900      |
| C41—H41A   | 1.0000      | C83—H83B    | 0.9900      |
| C42—H42A   | 0.9900      | C84—H84A    | 0.9900      |
| C42—H42B   | 0.9900      | C84—H84B    | 0.9900      |
| O1—Co1—O2  | 115.23 (5)  | O3—Co2—O4   | 114.40 (5)  |
| O1—Co1—N1  | 94.93 (5)   | O3—Co2—N3   | 94.94 (5)   |
| O2—Co1—N1  | 117.15 (5)  | O3—Co2—N4   | 116.97 (5)  |
| O1—Co1—N2  | 115.95 (5)  | O4—Co2—N3   | 115.20 (5)  |
| O2—Co1—N2  | 93.16 (5)   | O4—Co2—N4   | 94.63 (5)   |
| N1—Co1—N2  | 122.20 (6)  | N3—Co2—N4   | 122.25 (6)  |
| C22—O2—Co1 | 121.77 (11) | C43—O3—Co2  | 123.99 (10) |
| C1—O1—Co1  | 126.36 (11) | C64—O4—Co2  | 125.92 (11) |
| C11—N1—C12 | 119.94 (14) | C53—N3—C54  | 119.82 (13) |
| C11—N1—Co1 | 121.19 (11) | C53—N3—Co2  | 120.68 (11) |
| C12—N1—Co1 | 118.86 (10) | C54—N3—Co2  | 119.41 (10) |
| C32—N2—C33 | 120.42 (14) | C74—N4—C75  | 116.28 (13) |
| C32—N2—Co1 | 119.07 (11) | C74—N4—Co2  | 121.06 (11) |
| C33—N2—Co1 | 120.51 (10) | C75—N4—Co2  | 122.59 (10) |
| O1—C1—C10  | 124.93 (15) | O3—C43—C52  | 125.09 (15) |
| O1—C1—C2   | 116.18 (15) | O3—C43—C44  | 116.04 (15) |
| C10—C1—C2  | 118.88 (15) | C52—C43—C44 | 118.87 (15) |
| C3—C2—C1   | 121.71 (16) | C45—C44—C43 | 121.92 (16) |
| C3—C2—H2   | 119.1       | C45—C44—H44 | 119.0       |
| C1—C2—H2   | 119.1       | C43—C44—H44 | 119.0       |
| C2—C3—C4   | 121.53 (16) | C44—C45—C46 | 121.48 (16) |
| C2—C3—H3   | 119.2       | C44—C45—H45 | 119.3       |
| C4—C3—H3   | 119.2       | C46—C45—H45 | 119.3       |
| C5—C4—C9   | 120.22 (16) | C47—C46—C51 | 120.43 (15) |
| C5—C4—C3   | 120.82 (16) | C47—C46—C45 | 120.80 (15) |
| C9—C4—C3   | 118.94 (15) | C51—C46—C45 | 118.76 (15) |
| C6—C5—C4   | 121.44 (16) | C48—C47—C46 | 121.45 (16) |
| C6—C5—H5   | 119.3       | C48—C47—H47 | 119.3       |
| C4—C5—H5   | 119.3       | C46—C47—H47 | 119.3       |
| C5—C6—C7   | 119.04 (16) | C47—C48—C49 | 118.71 (16) |
| C5—C6—H6   | 120.5       | C47—C48—H48 | 120.6       |
| C7—C6—H6   | 120.5       | C49—C48—H48 | 120.6       |

## supplementary materials

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|               |             |               |             |
|---------------|-------------|---------------|-------------|
| C8—C7—C6      | 120.70 (17) | C50—C49—C48   | 121.30 (17) |
| C8—C7—H7      | 119.7       | C50—C49—H49   | 119.4       |
| C6—C7—H7      | 119.7       | C48—C49—H49   | 119.4       |
| C7—C8—C9      | 122.00 (16) | C49—C50—C51   | 121.70 (16) |
| C7—C8—H8      | 119.0       | C49—C50—H50   | 119.2       |
| C9—C8—H8      | 119.0       | C51—C50—H50   | 119.2       |
| C8—C9—C4      | 116.53 (15) | C50—C51—C46   | 116.39 (15) |
| C8—C9—C10     | 123.89 (15) | C50—C51—C52   | 123.94 (15) |
| C4—C9—C10     | 119.55 (15) | C46—C51—C52   | 119.66 (15) |
| C1—C10—C11    | 122.76 (15) | C43—C52—C53   | 122.64 (15) |
| C1—C10—C9     | 119.27 (15) | C43—C52—C51   | 119.27 (15) |
| C11—C10—C9    | 117.87 (15) | C53—C52—C51   | 118.01 (15) |
| N1—C11—C10    | 128.12 (16) | N3—C53—C52    | 127.69 (15) |
| N1—C11—H11    | 115.9       | N3—C53—H53    | 116.2       |
| C10—C11—H11   | 115.9       | C52—C53—H53   | 116.2       |
| N1—C12—C21    | 115.87 (13) | N3—C54—C55    | 115.18 (13) |
| N1—C12—C13    | 105.69 (13) | N3—C54—C59    | 107.40 (13) |
| C21—C12—C13   | 109.11 (14) | C55—C54—C59   | 108.96 (14) |
| N1—C12—C18    | 108.36 (13) | N3—C54—C63    | 107.59 (13) |
| C21—C12—C18   | 108.13 (14) | C55—C54—C63   | 108.29 (13) |
| C13—C12—C18   | 109.56 (14) | C59—C54—C63   | 109.32 (13) |
| C14—C13—C12   | 110.64 (14) | C54—C55—C56   | 109.89 (13) |
| C14—C13—H13A  | 109.5       | C54—C55—H55A  | 109.7       |
| C12—C13—H13A  | 109.5       | C56—C55—H55A  | 109.7       |
| C14—C13—H13B  | 109.5       | C54—C55—H55B  | 109.7       |
| C12—C13—H13B  | 109.5       | C56—C55—H55B  | 109.7       |
| H13A—C13—H13B | 108.1       | H55A—C55—H55B | 108.2       |
| C17—C14—C15   | 110.40 (16) | C57—C56—C60   | 110.09 (15) |
| C17—C14—C13   | 108.84 (15) | C57—C56—C55   | 109.65 (14) |
| C15—C14—C13   | 108.88 (15) | C60—C56—C55   | 109.34 (14) |
| C17—C14—H14   | 109.6       | C57—C56—H56   | 109.2       |
| C15—C14—H14   | 109.6       | C60—C56—H56   | 109.2       |
| C13—C14—H14   | 109.6       | C55—C56—H56   | 109.2       |
| C14—C15—C16   | 109.54 (15) | C56—C57—C58   | 109.03 (14) |
| C14—C15—H15A  | 109.8       | C56—C57—H57A  | 109.9       |
| C16—C15—H15A  | 109.8       | C58—C57—H57A  | 109.9       |
| C14—C15—H15B  | 109.8       | C56—C57—H57B  | 109.9       |
| C16—C15—H15B  | 109.8       | C58—C57—H57B  | 109.9       |
| H15A—C15—H15B | 108.2       | H57A—C57—H57B | 108.3       |
| C19—C16—C15   | 109.78 (16) | C62—C58—C57   | 109.56 (15) |
| C19—C16—C18   | 108.89 (15) | C62—C58—C59   | 109.35 (15) |
| C15—C16—C18   | 109.59 (15) | C57—C58—C59   | 109.30 (14) |
| C19—C16—H16   | 109.5       | C62—C58—H58   | 109.5       |
| C15—C16—H16   | 109.5       | C57—C58—H58   | 109.5       |
| C18—C16—H16   | 109.5       | C59—C58—H58   | 109.5       |
| C14—C17—C20   | 109.55 (15) | C54—C59—C58   | 110.28 (14) |
| C14—C17—H17A  | 109.8       | C54—C59—H59A  | 109.6       |
| C20—C17—H17A  | 109.8       | C58—C59—H59A  | 109.6       |
| C14—C17—H17B  | 109.8       | C54—C59—H59B  | 109.6       |

|               |             |               |             |
|---------------|-------------|---------------|-------------|
| C20—C17—H17B  | 109.8       | C58—C59—H59B  | 109.6       |
| H17A—C17—H17B | 108.2       | H59A—C59—H59B | 108.1       |
| C12—C18—C16   | 109.87 (14) | C61—C60—C56   | 109.07 (14) |
| C12—C18—H18A  | 109.7       | C61—C60—H60A  | 109.9       |
| C16—C18—H18A  | 109.7       | C56—C60—H60A  | 109.9       |
| C12—C18—H18B  | 109.7       | C61—C60—H60B  | 109.9       |
| C16—C18—H18B  | 109.7       | C56—C60—H60B  | 109.9       |
| H18A—C18—H18B | 108.2       | H60A—C60—H60B | 108.3       |
| C16—C19—C20   | 109.60 (15) | C60—C61—C63   | 109.44 (14) |
| C16—C19—H19A  | 109.7       | C60—C61—C62   | 109.29 (15) |
| C20—C19—H19A  | 109.7       | C63—C61—C62   | 109.75 (14) |
| C16—C19—H19B  | 109.7       | C60—C61—H61   | 109.5       |
| C20—C19—H19B  | 109.7       | C63—C61—H61   | 109.5       |
| H19A—C19—H19B | 108.2       | C62—C61—H61   | 109.5       |
| C17—C20—C19   | 109.64 (16) | C58—C62—C61   | 109.67 (14) |
| C17—C20—C21   | 109.43 (16) | C58—C62—H62A  | 109.7       |
| C19—C20—C21   | 109.43 (15) | C61—C62—H62A  | 109.7       |
| C17—C20—H20   | 109.4       | C58—C62—H62B  | 109.7       |
| C19—C20—H20   | 109.4       | C61—C62—H62B  | 109.7       |
| C21—C20—H20   | 109.4       | H62A—C62—H62B | 108.2       |
| C12—C21—C20   | 109.54 (14) | C61—C63—C54   | 110.17 (14) |
| C12—C21—H21A  | 109.8       | C61—C63—H63A  | 109.6       |
| C20—C21—H21A  | 109.8       | C54—C63—H63A  | 109.6       |
| C12—C21—H21B  | 109.8       | C61—C63—H63B  | 109.6       |
| C20—C21—H21B  | 109.8       | C54—C63—H63B  | 109.6       |
| H21A—C21—H21B | 108.2       | H63A—C63—H63B | 108.1       |
| O2—C22—C31    | 124.78 (15) | O4—C64—C73    | 124.69 (15) |
| O2—C22—C23    | 116.39 (15) | O4—C64—C65    | 116.66 (16) |
| C31—C22—C23   | 118.81 (16) | C73—C64—C65   | 118.63 (16) |
| C24—C23—C22   | 121.34 (17) | C66—C65—C64   | 121.26 (18) |
| C24—C23—H23   | 119.3       | C66—C65—H65   | 119.4       |
| C22—C23—H23   | 119.3       | C64—C65—H65   | 119.4       |
| C23—C24—C25   | 121.70 (17) | C65—C66—C67   | 122.16 (17) |
| C23—C24—H24   | 119.1       | C65—C66—H66   | 118.9       |
| C25—C24—H24   | 119.1       | C67—C66—H66   | 118.9       |
| C26—C25—C24   | 120.98 (16) | C68—C67—C66   | 121.41 (17) |
| C26—C25—C30   | 119.98 (17) | C68—C67—C72   | 119.76 (18) |
| C24—C25—C30   | 119.04 (16) | C66—C67—C72   | 118.79 (16) |
| C27—C26—C25   | 121.35 (17) | C69—C68—C67   | 121.75 (19) |
| C27—C26—H26   | 119.3       | C69—C68—H68   | 119.1       |
| C25—C26—H26   | 119.3       | C67—C68—H68   | 119.1       |
| C26—C27—C28   | 119.25 (17) | C68—C69—C70   | 118.81 (18) |
| C26—C27—H27   | 120.4       | C68—C69—H69   | 120.6       |
| C28—C27—H27   | 120.4       | C70—C69—H69   | 120.6       |
| C29—C28—C27   | 120.68 (18) | C71—C70—C69   | 121.1 (2)   |
| C29—C28—H28   | 119.7       | C71—C70—H70   | 119.5       |
| C27—C28—H28   | 119.7       | C69—C70—H70   | 119.5       |
| C28—C29—C30   | 121.78 (17) | C70—C71—C72   | 121.64 (19) |
| C28—C29—H29   | 119.1       | C70—C71—H71   | 119.2       |

## supplementary materials

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|               |             |               |             |
|---------------|-------------|---------------|-------------|
| C30—C29—H29   | 119.1       | C72—C71—H71   | 119.2       |
| C29—C30—C25   | 116.92 (16) | C71—C72—C67   | 116.92 (16) |
| C29—C30—C31   | 123.84 (16) | C71—C72—C73   | 123.71 (16) |
| C25—C30—C31   | 119.23 (16) | C67—C72—C73   | 119.34 (16) |
| C22—C31—C32   | 121.74 (15) | C64—C73—C74   | 122.65 (15) |
| C22—C31—C30   | 119.71 (15) | C64—C73—C72   | 119.65 (15) |
| C32—C31—C30   | 118.09 (15) | C74—C73—C72   | 117.69 (15) |
| N2—C32—C31    | 127.25 (16) | N4—C74—C73    | 128.48 (16) |
| N2—C32—H32    | 116.4       | N4—C74—H74    | 115.8       |
| C31—C32—H32   | 116.4       | C73—C74—H74   | 115.8       |
| N2—C33—C42    | 115.05 (13) | N4—C75—C80    | 108.12 (13) |
| N2—C33—C34    | 107.43 (13) | N4—C75—C84    | 112.62 (13) |
| C42—C33—C34   | 108.71 (14) | C80—C75—C84   | 108.37 (13) |
| N2—C33—C38    | 107.47 (13) | N4—C75—C76    | 109.25 (13) |
| C42—C33—C38   | 108.98 (14) | C80—C75—C76   | 108.52 (13) |
| C34—C33—C38   | 109.06 (13) | C84—C75—C76   | 109.87 (14) |
| C35—C34—C33   | 110.33 (14) | C77—C76—C75   | 110.22 (13) |
| C35—C34—H34A  | 109.6       | C77—C76—H76A  | 109.6       |
| C33—C34—H34A  | 109.6       | C75—C76—H76A  | 109.6       |
| C35—C34—H34B  | 109.6       | C77—C76—H76B  | 109.6       |
| C33—C34—H34B  | 109.6       | C75—C76—H76B  | 109.6       |
| H34A—C34—H34B | 108.1       | H76A—C76—H76B | 108.1       |
| C39—C35—C34   | 109.61 (15) | C78—C77—C83   | 109.92 (14) |
| C39—C35—C36   | 109.33 (16) | C78—C77—C76   | 108.90 (14) |
| C34—C35—C36   | 109.37 (15) | C83—C77—C76   | 109.11 (14) |
| C39—C35—H35   | 109.5       | C78—C77—H77   | 109.6       |
| C34—C35—H35   | 109.5       | C83—C77—H77   | 109.6       |
| C36—C35—H35   | 109.5       | C76—C77—H77   | 109.6       |
| C37—C36—C35   | 109.23 (14) | C77—C78—C79   | 109.62 (14) |
| C37—C36—H36A  | 109.8       | C77—C78—H78A  | 109.7       |
| C35—C36—H36A  | 109.8       | C79—C78—H78A  | 109.7       |
| C37—C36—H36B  | 109.8       | C77—C78—H78B  | 109.7       |
| C35—C36—H36B  | 109.8       | C79—C78—H78B  | 109.7       |
| H36A—C36—H36B | 108.3       | H78A—C78—H78B | 108.2       |
| C40—C37—C36   | 109.98 (15) | C81—C79—C78   | 109.46 (15) |
| C40—C37—C38   | 109.15 (15) | C81—C79—C80   | 109.03 (14) |
| C36—C37—C38   | 109.70 (15) | C78—C79—C80   | 109.51 (14) |
| C40—C37—H37   | 109.3       | C81—C79—H79   | 109.6       |
| C36—C37—H37   | 109.3       | C78—C79—H79   | 109.6       |
| C38—C37—H37   | 109.3       | C80—C79—H79   | 109.6       |
| C33—C38—C37   | 109.75 (14) | C75—C80—C79   | 110.57 (14) |
| C33—C38—H38A  | 109.7       | C75—C80—H80A  | 109.5       |
| C37—C38—H38A  | 109.7       | C79—C80—H80A  | 109.5       |
| C33—C38—H38B  | 109.7       | C75—C80—H80B  | 109.5       |
| C37—C38—H38B  | 109.7       | C79—C80—H80B  | 109.5       |
| H38A—C38—H38B | 108.2       | H80A—C80—H80B | 108.1       |
| C41—C39—C35   | 109.38 (15) | C79—C81—C82   | 109.61 (14) |
| C41—C39—H39A  | 109.8       | C79—C81—H81A  | 109.7       |
| C35—C39—H39A  | 109.8       | C82—C81—H81A  | 109.7       |



|               |             |               |             |
|---------------|-------------|---------------|-------------|
| C41—C39—H39B  | 109.8       | C79—C81—H81B  | 109.7       |
| C35—C39—H39B  | 109.8       | C82—C81—H81B  | 109.7       |
| H39A—C39—H39B | 108.2       | H81A—C81—H81B | 108.2       |
| C37—C40—C41   | 109.28 (15) | C83—C82—C81   | 109.61 (15) |
| C37—C40—H40A  | 109.8       | C83—C82—C84   | 109.54 (15) |
| C41—C40—H40A  | 109.8       | C81—C82—C84   | 109.31 (15) |
| C37—C40—H40B  | 109.8       | C83—C82—H82   | 109.5       |
| C41—C40—H40B  | 109.8       | C81—C82—H82   | 109.5       |
| H40A—C40—H40B | 108.3       | C84—C82—H82   | 109.5       |
| C39—C41—C40   | 109.48 (15) | C82—C83—C77   | 109.77 (14) |
| C39—C41—C42   | 109.80 (16) | C82—C83—H83A  | 109.7       |
| C40—C41—C42   | 109.43 (15) | C77—C83—H83A  | 109.7       |
| C39—C41—H41A  | 109.4       | C82—C83—H83B  | 109.7       |
| C40—C41—H41A  | 109.4       | C77—C83—H83B  | 109.7       |
| C42—C41—H41A  | 109.4       | H83A—C83—H83B | 108.2       |
| C33—C42—C41   | 109.89 (14) | C75—C84—C82   | 109.50 (14) |
| C33—C42—H42A  | 109.7       | C75—C84—H84A  | 109.8       |
| C41—C42—H42A  | 109.7       | C82—C84—H84A  | 109.8       |
| C33—C42—H42B  | 109.7       | C75—C84—H84B  | 109.8       |
| C41—C42—H42B  | 109.7       | C82—C84—H84B  | 109.8       |
| H42A—C42—H42B | 108.2       | H84A—C84—H84B | 108.2       |

Fig. 1

