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

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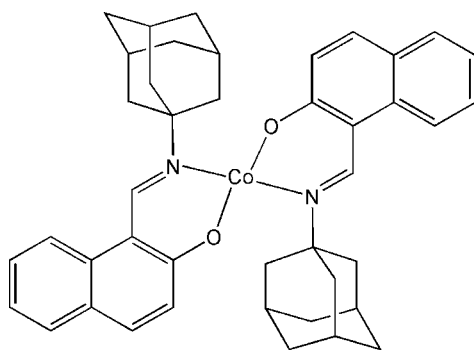
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 Key indicators: single-crystal X-ray study; $T = 90$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.036; wR factor = 0.088; data-to-parameter ratio = 18.0.

The title compound, $[\text{Co}(\text{C}_{21}\text{H}_{22}\text{NO})_2]$, 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

 $[\text{Co}(\text{C}_{21}\text{H}_{22}\text{NO})_2]$
 $M_r = 667.72$

 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) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.56$ mm⁻¹
 $T = 90$ (2) K
 $0.33 \times 0.24 \times 0.18$ mm

Data collection

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

 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⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³
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.

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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.

supporting information

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

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

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S1. Comment

The title Co^{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-Cu^{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 Co^{II} is in the normal range for complexes of this type. The N₂O₂ donor set forms a distorted tetrahedral coordination with angles at Co ranging from 93.16 (5)° to 122.20 (6)° in the complex involving Co1 and 94.63 (5)° to 122.25 (6)° 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.

S2. 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 CoCl₂·2(H₂O) (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%.

S3. 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 $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

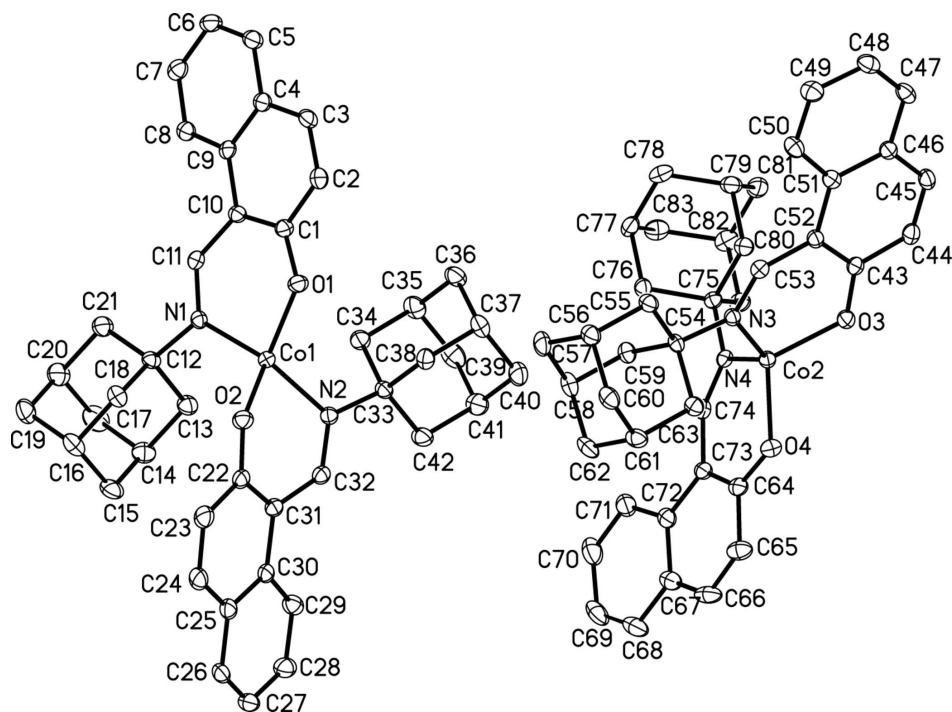


Figure 1

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.

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Crystal data

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Triclinic, $P\bar{1}$

Hall symbol: -P 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) Å³

$Z = 4$

$F(000) = 1412$

$D_x = 1.332$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5583 reflections

$\theta = 2.8\text{--}27.4^\circ$

$\mu = 0.56$ mm⁻¹

$T = 90$ 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

Graphite monochromator

Detector resolution: 8.3 pixels mm⁻¹

ω 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 $I > 2\sigma(I)$

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

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.8^\circ$

$h = -18 \rightarrow 18$

$k = -18 \rightarrow 18$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.088$
 $S = 1.02$
 15246 reflections
 847 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 1.0354P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

Special details

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

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 (\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* |
| 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) |
| 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 (\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) |
| 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) |
| 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) |

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| 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 |

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| 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 |
| 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 |

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| 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) |

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| 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 |
| 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) |

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| 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 |