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# Acrylato[tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine]cobalt(II) perchlorate–dimethylformamide–methanol (2/2/3)

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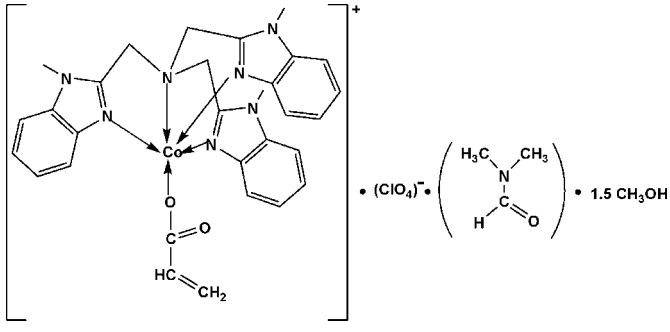
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.046; $wR$ factor = 0.147; data-to-parameter ratio = 13.5.

In the title complex, $[Co(C_3H_3O_2)(C_{27}H_{27}N_7)]ClO_4\cdot C_3H_7NO\cdot 1.5CH_4O$, the $Co^{II}$ ion is five-coordinated by four N atoms from a tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine (mentb) ligand and one O atom from an acrylate ligand in a distorted trigonal–bipyramidal geometry with approximate molecular $C_3$ symmetry. The atoms of the acrylate ligand are disordered over two sites, with approximate occupancies of 0.90 and 0.10. In addition, the solvent hemimethanol molecule is disordered over two positions with equal occupancies. The crystal structure is stabilized by weak intermolecular O—H···O hydrogen bonds.

## Related literature

For background information, see: Youngme *et al.* (2007). For bond-length data, see: Allen *et al.* (1987).



## Experimental

### Crystal data

$[Co(C_3H_3O_2)(C_{27}H_{27}N_7)]ClO_4\cdot C_3H_7NO\cdot 1.5CH_4O$
$M_r$ = 800.15
Triclinic, $P\overline{1}$
$a$ = 11.3398 (3) Å
$b$ = 13.9507 (4) Å
$c$ = 14.4270 (5) Å
$\alpha$ = 108.443 (1)°
$\beta$ = 110.738 (1)°
$\gamma$ = 100.278 (1)°
$V$ = 1913.24 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.58 mm$^{-1}$
$T$ = 153 (2) K
0.35 × 0.32 × 0.26 mm

### Data collection

Rigaku R-AXIS Spider diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.823, $T_{max}$ = 0.864
15711 measured reflections
7032 independent reflections
6085 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.147
$S$ = 1.07
7032 reflections
519 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O8—H8O···O7$^{i}$ | 0.84 | 1.94 | 2.765 (4) | 169 |

Symmetry code: (i) $-x+2, -y+2, -z+1$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2706).

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# supporting information

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# Acrylato[tris(1-methyl-1*H*-benzimidazol-2-ylmethyl)amine]cobalt(II) perchlorate–dimethylformamide–methanol (2/2/3)

**Huilu Wu, Wei Ying, Kaitong Wang, Xingcai Huang and Ke Li**

## S1. Comment

The asymmetric unit of the title compound (I), (Fig. 1), consists of a discrete [Co(mentb)(acrylate)] cation, a perchlorate anion, a DMF molecule and 1.5 molecules of methanol. The cobalt ion is five-coordinate with a $N_4O$ ligand set. The mentb ligand acts as a tetradentate N-donor, and an O atom of the carboxylate group of the acrylate ligand completes the coordination. The coordination geometry of the $Co^{II}$ ion may be best described as distorted trigonal bipyramidal ($\tau$ = 0.87), with approximate site symmetry $C_3$. The parameter $\tau$ is defined as ($\beta$ - $\alpha$)/60 [where $\beta$ = O1—Co—N7, $\alpha$ = N3—Co —N5] and its value varies from 0 (in regular square-based pyramidal) to 1 (in regular trigonal bipyramidal) [Youngme *et al.*, 2007]. This geometry is assumed by the $Co^{II}$ ion presumably to relieve the steric crowding. The equatorial plane is occupied by three N atoms of three benzimidazolyl groups, while the $Co^{II}$ ion protrudes towards atom O1 and is 0.528 (2) Å from the plane of atoms N1/N3/N5. The axial positions are occupied by atoms N7 and O1. The three benzimidazole ring arms of the mentb ligand form a cone-shaped cavity. The distance between $Co^{II}$ and O2 is 3.076 (2) A, so atom O2 is not considered to be coordinated. The angles and distances in the mentb and salicylate are normally equal [for standard bond lengths, see: Allen *et al.*, 1987]. The crystal structure is stabilized by weak intermolecular O-H···O hydrogen bonds and weak $\pi$···$\pi$ stacking interactions (Fig. 2). The significant stacking interactions have ring centroid···ring centroid distances in the range 3.456 (2)-3.646 (2)Å.

## S2. Experimental

To a stirred solution of tris(1-methyl-1H-benzimidazol-2-ylmethyl)amine (0.0899 g, 0.2 mmol) in hot MeOH (10 ml) was added $Co(ClO_4)_2$ $(H_2O)_6$ (0.0732 g, 0.2 mmol), followed by a solution of Na(acrylate) (0.0188 g, 0.2 mmol) in MeOH (5 ml). A red crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute $Et_2O$, and dried *in vacuo*. The dried precipitate was dissolved in DMF to a red solution that was allowed to evaporate at room temperature. The red crystals suitable for X-ray diffraction studies were obtained after four weeks. Yield, 0.106 g (66%). (found: C, 51.67; H, 5.38; N,14.21. Calcd. for C34.50H43ClN8O8.50Co: C, 51.79; H, 5.42; N, 14.00)

## S3. Refinement

All H atoms were found in difference electron maps and were subsequently refined in a riding-model approximation with C—H distances ranging from 0.95 to 0.99 Å and O—H distance 0.84 Å and $U_{iso}$(H) = 1.2 $U_{eq}$ of the carrier atom,

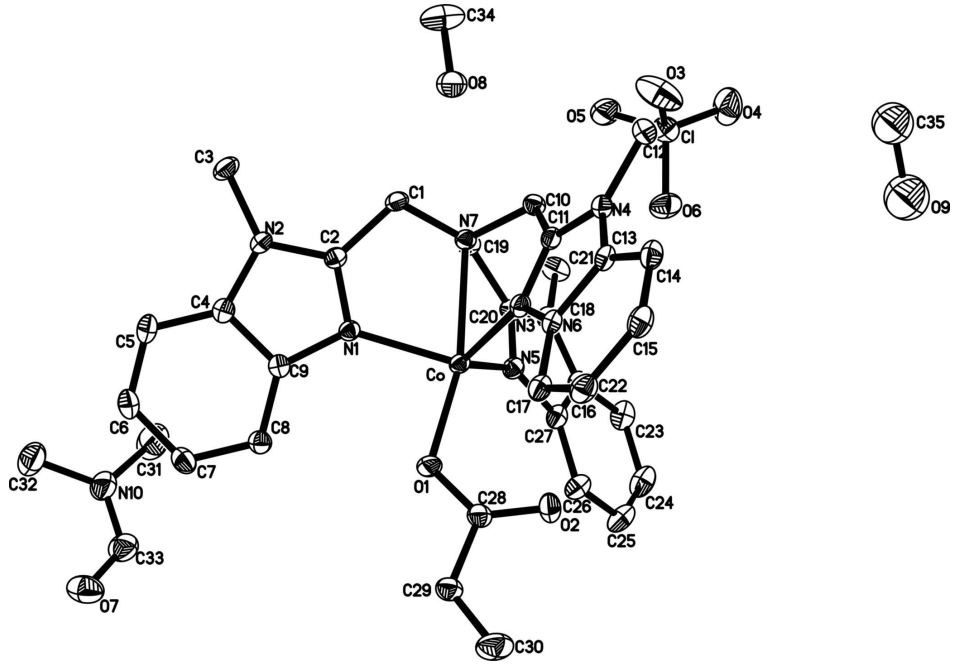


**Figure 1**

Molecular structure and atom numbering for the components of (I). Hydrogen atoms have been omitted for clarity and the displacement ellipsoids are shown at the 30% probability level.

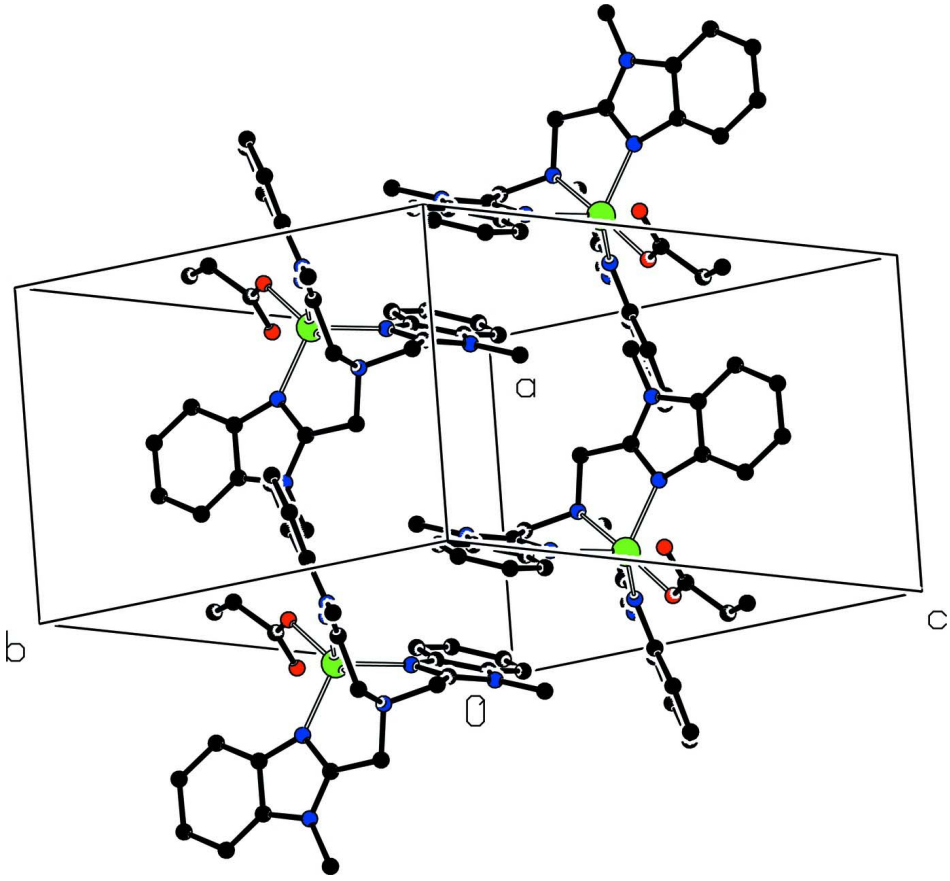


**Figure 2**

The packing of the cations. Neither the disorder or H atoms are shown.

**Acrylato[tris(1-methyl-1H-benzimidazol-2-ylmethyl)amine]cobalt(II) perchlorate–dimethylformamide–methanol (2/2/3)**

*Crystal data*

$[Co(C_3H_3O_2)(C_{27}H_{27}N_7)]ClO_4·C_3H_7NO·1.5CH_4O$
$M_r$ = 800.15
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 11.3398 (3) Å
$b$ = 13.9507 (4) Å
$c$ = 14.4270 (5) Å
$\alpha$ = 108.443 (1)°
$\beta$ = 110.738 (1)°
$\gamma$ = 100.278 (1)°
$V$ = 1913.24 (10) Å$^3$
$Z$ = 2
$F$(000) = 836
$D_x$ = 1.389 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 7032 reflections
$\theta$ = 3.0–25.5°
$\mu$ = 0.58 mm$^{-1}$
$T$ = 153 K
Block, red
0.35 × 0.32 × 0.26 mm

*Data collection*

Rigaku R-AXIS Spider diffractometer
Radiation source: Rotating Anode
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.823, $T_{max}$ = 0.864
15711 measured reflections
7032 independent reflections

6085 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 13$
$k = -15 \rightarrow 16$
$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.147$
$S = 1.07$
7032 reflections
519 parameters
6 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
$w = 1/[\sigma^2(F_o^2) + (0.0954P)^2 + 1.1776P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.26$ e Å$^{-3}$
$\Delta\rho_{min} = -0.44$ e Å$^{-3}$

*Special details*

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

**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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Co | 0.85373 (3) | 0.66082 (3) | 0.32233 (3) | 0.02259 (13) | |
| Cl | 0.39694 (7) | 0.32230 (6) | 0.32447 (6) | 0.03835 (19) | |
| O1 | 0.9876 (2) | 0.71250 (18) | 0.27486 (15) | 0.0330 (7) | 0.901 (5) |
| O2 | 0.9039 (2) | 0.56682 (14) | 0.12161 (16) | 0.0361 (7) | 0.901 (5) |
| O1′ | 0.932 (2) | 0.6236 (16) | 0.2363 (16) | 0.044 (7) | 0.099 (5) |
| O2′ | 0.986 (3) | 0.7549 (7) | 0.218 (3) | 0.13 (2) | 0.099 (5) |
| O3 | 0.3275 (3) | 0.3884 (3) | 0.2891 (3) | 0.0793 (10) | |
| O4 | 0.3064 (3) | 0.2197 (2) | 0.2890 (2) | 0.0725 (8) | |
| O5 | 0.4629 (2) | 0.3703 (2) | 0.4417 (2) | 0.0591 (7) | |
| O6 | 0.4972 (2) | 0.3160 (2) | 0.28583 (19) | 0.0499 (6) | |
| O7 | 1.6359 (3) | 1.0565 (2) | 0.7244 (3) | 0.0626 (7) | |
| O8 | 0.4466 (2) | 0.78673 (17) | 0.33218 (19) | 0.0411 (5) | |
| H8O | 0.4266 | 0.8330 | 0.3098 | 0.049* | |
| N1 | 0.9381 (2) | 0.79702 (17) | 0.46404 (16) | 0.0234 (4) | |
| N2 | 0.9256 (2) | 0.91605 (17) | 0.60230 (17) | 0.0261 (5) | |
| N3 | 0.6689 (2) | 0.64681 (16) | 0.21381 (16) | 0.0240 (4) | |
| N4 | 0.4473 (2) | 0.58321 (17) | 0.14350 (17) | 0.0259 (5) | |
| N5 | 0.8638 (2) | 0.52411 (17) | 0.34938 (17) | 0.0263 (5) | |
| N6 | 0.8178 (2) | 0.41123 (19) | 0.42099 (18) | 0.0301 (5) | |
| N7 | 0.7151 (2) | 0.64080 (17) | 0.40828 (17) | 0.0238 (4) | |
| N10 | 1.5434 (3) | 1.0109 (2) | 0.8268 (3) | 0.0549 (8) | |
| C1 | 0.7256 (2) | 0.7501 (2) | 0.4742 (2) | 0.0272 (5) | |

| | | | | |
|---|---|---|---|---|
| H1A | 0.7061 | 0.7509 | 0.5360 | 0.033* |
| H1B | 0.6607 | 0.7750 | 0.4293 | 0.033* |
| C2 | 0.8638 (2) | 0.8210 (2) | 0.5149 (2) | 0.0241 (5) |
| C3 | 0.8707 (3) | 0.9685 (2) | 0.6741 (2) | 0.0366 (7) |
| H3A | 0.7731 | 0.9378 | 0.6375 | 0.044* |
| H3B | 0.8970 | 1.0453 | 0.6917 | 0.044* |
| H3C | 0.9051 | 0.9577 | 0.7413 | 0.044* |
| C4 | 1.0501 (3) | 0.9576 (2) | 0.6089 (2) | 0.0269 (5) |
| C5 | 1.1554 (3) | 1.0522 (2) | 0.6819 (2) | 0.0345 (6) |
| H5 | 1.1500 | 1.1030 | 0.7409 | 0.041* |
| C6 | 1.2672 (3) | 1.0684 (2) | 0.6645 (2) | 0.0373 (7) |
| H6 | 1.3411 | 1.1318 | 0.7131 | 0.045* |
| C7 | 1.2759 (3) | 0.9943 (2) | 0.5770 (3) | 0.0360 (6) |
| H7 | 1.3548 | 1.0088 | 0.5674 | 0.043* |
| C8 | 1.1712 (3) | 0.9002 (2) | 0.5046 (2) | 0.0283 (6) |
| H8 | 1.1770 | 0.8496 | 0.4456 | 0.034* |
| C9 | 1.0573 (2) | 0.8826 (2) | 0.5214 (2) | 0.0238 (5) |
| C10 | 0.5791 (2) | 0.5790 (2) | 0.3218 (2) | 0.0260 (5) |
| H10A | 0.5129 | 0.5983 | 0.3475 | 0.031* |
| H10B | 0.5637 | 0.5015 | 0.3013 | 0.031* |
| C11 | 0.5648 (2) | 0.60425 (19) | 0.2267 (2) | 0.0240 (5) |
| C12 | 0.3149 (3) | 0.5384 (2) | 0.1345 (2) | 0.0318 (6) |
| H12A | 0.3172 | 0.4867 | 0.1673 | 0.038* |
| H12B | 0.2503 | 0.5025 | 0.0576 | 0.038* |
| H12C | 0.2885 | 0.5960 | 0.1726 | 0.038* |
| C13 | 0.4752 (3) | 0.61622 (19) | 0.0702 (2) | 0.0256 (5) |
| C14 | 0.3922 (3) | 0.6132 (2) | −0.0293 (2) | 0.0308 (6) |
| H14 | 0.2978 | 0.5849 | −0.0592 | 0.037* |
| C15 | 0.4537 (3) | 0.6533 (2) | −0.0823 (2) | 0.0334 (6) |
| H15 | 0.4005 | 0.6532 | −0.1501 | 0.040* |
| C16 | 0.5937 (3) | 0.6943 (2) | −0.0384 (2) | 0.0332 (6) |
| H16 | 0.6326 | 0.7216 | −0.0772 | 0.040* |
| C17 | 0.6760 (3) | 0.6959 (2) | 0.0598 (2) | 0.0296 (6) |
| H17 | 0.7704 | 0.7231 | 0.0887 | 0.036* |
| C18 | 0.6152 (2) | 0.65610 (19) | 0.11455 (19) | 0.0233 (5) |
| C19 | 0.7642 (3) | 0.5831 (2) | 0.4753 (2) | 0.0283 (6) |
| H19A | 0.6911 | 0.5449 | 0.4859 | 0.034* |
| H19B | 0.8366 | 0.6338 | 0.5475 | 0.034* |
| C20 | 0.8152 (2) | 0.5053 (2) | 0.4155 (2) | 0.0263 (5) |
| C21 | 0.7751 (3) | 0.3659 (3) | 0.4873 (3) | 0.0378 (7) |
| H21A | 0.7347 | 0.4119 | 0.5237 | 0.045* |
| H21B | 0.8526 | 0.3613 | 0.5420 | 0.045* |
| H21C | 0.7096 | 0.2942 | 0.4404 | 0.045* |
| C22 | 0.8701 (3) | 0.3637 (2) | 0.3524 (2) | 0.0312 (6) |
| C23 | 0.8903 (3) | 0.2653 (2) | 0.3241 (2) | 0.0393 (7) |
| H23 | 0.8661 | 0.2158 | 0.3521 | 0.047* |
| C24 | 0.9470 (3) | 0.2433 (3) | 0.2537 (3) | 0.0450 (8) |
| H24 | 0.9626 | 0.1768 | 0.2324 | 0.054* |

| | | | | | |
|---|---|---|---|---|---|
| C25 | 0.9826 (3) | 0.3152 (3) | 0.2123 (2) | 0.0429 (8) | |
| H25 | 1.0239 | 0.2975 | 0.1652 | 0.051* | |
| C26 | 0.9593 (3) | 0.4119 (2) | 0.2381 (2) | 0.0342 (6) | |
| H26 | 0.9823 | 0.4604 | 0.2087 | 0.041* | |
| C27 | 0.9011 (3) | 0.4354 (2) | 0.3086 (2) | 0.0283 (6) | |
| C28 | 0.9799 (2) | 0.65979 (16) | 0.18204 (15) | 0.0300 (6) | |
| C29 | 1.0710 (3) | 0.7152 (3) | 0.1482 (3) | 0.0325 (8) | 0.901 (5) |
| H29 | 1.1327 | 0.7843 | 0.1984 | 0.039* | 0.901 (5) |
| C29′ | 1.036 (4) | 0.643 (5) | 0.120 (4) | 0.055 (11) | 0.099 (5) |
| H29′ | 1.0652 | 0.5833 | 0.1212 | 0.066* | 0.099 (5) |
| C30 | 1.0707 (4) | 0.6743 (3) | 0.0539 (3) | 0.0543 (9) | |
| H30A | 1.0100 | 0.6053 | 0.0021 | 0.065* | |
| H30B | 1.1311 | 0.7133 | 0.0366 | 0.065* | |
| C31 | 1.4675 (7) | 0.9251 (4) | 0.8413 (5) | 0.102 (2) | |
| H31A | 1.4460 | 0.8564 | 0.7820 | 0.122* | |
| H31B | 1.3847 | 0.9373 | 0.8404 | 0.122* | |
| H31C | 1.5208 | 0.9242 | 0.9110 | 0.122* | |
| C32 | 1.5733 (5) | 1.1192 (3) | 0.9011 (4) | 0.0640 (11) | |
| H32A | 1.6163 | 1.1692 | 0.8788 | 0.077* | |
| H32B | 1.6334 | 1.1307 | 0.9748 | 0.077* | |
| H32C | 1.4904 | 1.1312 | 0.9002 | 0.077* | |
| C33 | 1.5787 (4) | 0.9898 (3) | 0.7467 (3) | 0.0533 (9) | |
| H33 | 1.5583 | 0.9167 | 0.7023 | 0.064* | |
| C34 | 0.3940 (4) | 0.7816 (4) | 0.4049 (4) | 0.0641 (11) | |
| H34A | 0.4298 | 0.7369 | 0.4403 | 0.077* | |
| H34B | 0.2966 | 0.7505 | 0.3654 | 0.077* | |
| H34C | 0.4186 | 0.8538 | 0.4600 | 0.077* | |
| C35 | 0.103 (2) | 0.0960 (19) | 0.008 (2) | 0.097 (5)* | 0.25 |
| H35A | 0.1537 | 0.1582 | 0.0783 | 0.116* | 0.25 |
| H35B | 0.0371 | 0.0450 | 0.0143 | 0.116* | 0.25 |
| H35C | 0.0562 | 0.1191 | −0.0477 | 0.116* | 0.25 |
| O9 | 0.192 (2) | 0.0453 (16) | −0.0210 (17) | 0.119 (6)* | 0.25 |
| H9O | 0.1654 | −0.0198 | −0.0342 | 0.143* | 0.25 |
| O9′ | 0.0197 (16) | −0.0281 (13) | −0.0351 (13) | 0.103 (5)* | 0.25 |
| H9O′ | −0.0390 | −0.0076 | −0.0706 | 0.123* | 0.25 |
| C35′ | 0.1498 (19) | 0.0451 (19) | 0.001 (2) | 0.097 (5)* | 0.25 |
| H35D | 0.1991 | 0.0079 | −0.0330 | 0.116* | 0.25 |
| H35E | 0.1986 | 0.0723 | 0.0804 | 0.116* | 0.25 |
| H35F | 0.1403 | 0.1049 | −0.0192 | 0.116* | 0.25 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co | 0.0241 (2) | 0.0256 (2) | 0.01876 (19) | 0.00885 (15) | 0.01064 (14) | 0.00814 (15) |
| Cl | 0.0424 (4) | 0.0413 (4) | 0.0393 (4) | 0.0115 (3) | 0.0212 (3) | 0.0237 (3) |
| O1 | 0.0313 (11) | 0.0420 (16) | 0.0238 (12) | 0.0071 (10) | 0.0163 (9) | 0.0093 (10) |
| O2 | 0.0368 (12) | 0.0301 (12) | 0.0278 (12) | 0.0009 (10) | 0.0079 (9) | 0.0081 (10) |
| O1′ | 0.047 (13) | 0.025 (13) | 0.070 (17) | 0.016 (10) | 0.028 (12) | 0.028 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O2′ | 0.041 (16) | 0.22 (5) | 0.034 (18) | −0.03 (2) | 0.002 (13) | 0.00 (3) |
| O3 | 0.0489 (15) | 0.098 (2) | 0.131 (3) | 0.0352 (16) | 0.0395 (17) | 0.089 (2) |
| O4 | 0.093 (2) | 0.0444 (15) | 0.0691 (19) | −0.0045 (14) | 0.0426 (17) | 0.0164 (13) |
| O5 | 0.0536 (14) | 0.0789 (18) | 0.0389 (13) | 0.0181 (13) | 0.0253 (11) | 0.0135 (13) |
| O6 | 0.0583 (14) | 0.0663 (16) | 0.0415 (13) | 0.0240 (12) | 0.0330 (11) | 0.0274 (12) |
| O7 | 0.0648 (16) | 0.0669 (17) | 0.093 (2) | 0.0363 (14) | 0.0515 (16) | 0.0508 (16) |
| O8 | 0.0404 (11) | 0.0401 (12) | 0.0503 (13) | 0.0156 (10) | 0.0258 (10) | 0.0196 (10) |
| N1 | 0.0243 (10) | 0.0256 (11) | 0.0207 (10) | 0.0088 (9) | 0.0105 (8) | 0.0091 (9) |
| N2 | 0.0313 (11) | 0.0252 (11) | 0.0237 (11) | 0.0114 (9) | 0.0145 (9) | 0.0085 (9) |
| N3 | 0.0266 (10) | 0.0237 (11) | 0.0188 (10) | 0.0068 (9) | 0.0090 (8) | 0.0072 (8) |
| N4 | 0.0244 (10) | 0.0252 (11) | 0.0228 (11) | 0.0064 (9) | 0.0084 (9) | 0.0066 (9) |
| N5 | 0.0277 (11) | 0.0273 (11) | 0.0240 (11) | 0.0110 (9) | 0.0108 (9) | 0.0102 (9) |
| N6 | 0.0313 (11) | 0.0347 (12) | 0.0279 (12) | 0.0128 (10) | 0.0110 (9) | 0.0184 (10) |
| N7 | 0.0230 (10) | 0.0272 (11) | 0.0215 (10) | 0.0085 (9) | 0.0101 (8) | 0.0096 (9) |
| N10 | 0.069 (2) | 0.0374 (15) | 0.062 (2) | 0.0160 (14) | 0.0381 (17) | 0.0153 (14) |
| C1 | 0.0267 (12) | 0.0308 (14) | 0.0262 (13) | 0.0126 (11) | 0.0151 (11) | 0.0089 (11) |
| C2 | 0.0267 (12) | 0.0269 (13) | 0.0214 (12) | 0.0109 (10) | 0.0113 (10) | 0.0112 (10) |
| C3 | 0.0473 (17) | 0.0342 (15) | 0.0338 (15) | 0.0167 (13) | 0.0264 (13) | 0.0090 (12) |
| C4 | 0.0316 (13) | 0.0245 (13) | 0.0268 (13) | 0.0109 (11) | 0.0117 (11) | 0.0134 (11) |
| C5 | 0.0442 (16) | 0.0217 (13) | 0.0295 (14) | 0.0074 (12) | 0.0126 (12) | 0.0064 (11) |
| C6 | 0.0383 (15) | 0.0247 (14) | 0.0377 (16) | 0.0017 (12) | 0.0117 (13) | 0.0099 (12) |
| C7 | 0.0310 (14) | 0.0309 (15) | 0.0452 (17) | 0.0062 (12) | 0.0160 (13) | 0.0175 (13) |
| C8 | 0.0297 (13) | 0.0266 (13) | 0.0314 (14) | 0.0098 (11) | 0.0145 (11) | 0.0140 (11) |
| C9 | 0.0257 (12) | 0.0235 (12) | 0.0233 (12) | 0.0085 (10) | 0.0089 (10) | 0.0129 (10) |
| C10 | 0.0241 (12) | 0.0290 (13) | 0.0254 (13) | 0.0075 (10) | 0.0115 (10) | 0.0120 (11) |
| C11 | 0.0250 (12) | 0.0209 (12) | 0.0223 (12) | 0.0075 (10) | 0.0092 (10) | 0.0058 (10) |
| C12 | 0.0261 (13) | 0.0324 (14) | 0.0308 (14) | 0.0065 (11) | 0.0097 (11) | 0.0104 (12) |
| C13 | 0.0309 (13) | 0.0190 (12) | 0.0222 (12) | 0.0080 (10) | 0.0101 (10) | 0.0047 (10) |
| C14 | 0.0316 (13) | 0.0274 (14) | 0.0229 (13) | 0.0095 (11) | 0.0054 (11) | 0.0050 (11) |
| C15 | 0.0416 (15) | 0.0335 (15) | 0.0196 (13) | 0.0139 (12) | 0.0080 (11) | 0.0096 (11) |
| C16 | 0.0428 (15) | 0.0335 (15) | 0.0253 (14) | 0.0126 (12) | 0.0167 (12) | 0.0127 (12) |
| C17 | 0.0328 (13) | 0.0280 (13) | 0.0231 (13) | 0.0090 (11) | 0.0113 (11) | 0.0061 (11) |
| C18 | 0.0272 (12) | 0.0201 (12) | 0.0183 (12) | 0.0073 (10) | 0.0084 (10) | 0.0047 (10) |
| C19 | 0.0304 (13) | 0.0337 (14) | 0.0246 (13) | 0.0112 (11) | 0.0137 (11) | 0.0143 (11) |
| C20 | 0.0232 (12) | 0.0333 (14) | 0.0235 (12) | 0.0100 (11) | 0.0085 (10) | 0.0145 (11) |
| C21 | 0.0373 (15) | 0.0484 (18) | 0.0414 (17) | 0.0171 (13) | 0.0180 (13) | 0.0324 (15) |
| C22 | 0.0299 (13) | 0.0350 (15) | 0.0248 (13) | 0.0121 (12) | 0.0058 (11) | 0.0141 (12) |
| C23 | 0.0465 (17) | 0.0358 (16) | 0.0332 (15) | 0.0196 (14) | 0.0088 (13) | 0.0179 (13) |
| C24 | 0.060 (2) | 0.0393 (17) | 0.0343 (16) | 0.0317 (16) | 0.0127 (15) | 0.0139 (14) |
| C25 | 0.0554 (19) | 0.0497 (18) | 0.0280 (15) | 0.0328 (16) | 0.0175 (14) | 0.0138 (14) |
| C26 | 0.0420 (15) | 0.0389 (16) | 0.0276 (14) | 0.0224 (13) | 0.0157 (12) | 0.0153 (12) |
| C27 | 0.0288 (13) | 0.0289 (13) | 0.0233 (13) | 0.0131 (11) | 0.0065 (10) | 0.0095 (11) |
| C28 | 0.0235 (13) | 0.0390 (16) | 0.0241 (14) | 0.0085 (12) | 0.0083 (11) | 0.0120 (13) |
| C29 | 0.0312 (17) | 0.037 (2) | 0.0329 (17) | 0.0101 (15) | 0.0172 (14) | 0.0168 (16) |
| C29′ | 0.039 (19) | 0.08 (3) | 0.09 (3) | 0.04 (2) | 0.04 (2) | 0.06 (3) |
| C30 | 0.058 (2) | 0.076 (3) | 0.0445 (19) | 0.0227 (19) | 0.0338 (17) | 0.0312 (19) |
| C31 | 0.159 (6) | 0.052 (3) | 0.113 (4) | 0.012 (3) | 0.100 (4) | 0.023 (3) |
| C32 | 0.079 (3) | 0.045 (2) | 0.063 (2) | 0.0224 (19) | 0.033 (2) | 0.0117 (18) |

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|---|---|---|---|---|---|---|
| C33 | 0.061 (2) | 0.047 (2) | 0.064 (2) | 0.0267 (18) | 0.0360 (19) | 0.0236 (18) |
| C34 | 0.065 (2) | 0.094 (3) | 0.070 (3) | 0.049 (2) | 0.049 (2) | 0.045 (2) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Co—O1′ | 1.772 (13) | C12—H12A | 0.9800 |
| Co—O1 | 1.988 (2) | C12—H12B | 0.9800 |
| Co—N1 | 2.053 (2) | C12—H12C | 0.9800 |
| Co—N3 | 2.054 (2) | C13—C14 | 1.393 (4) |
| Co—N5 | 2.078 (2) | C13—C18 | 1.407 (4) |
| Co—N7 | 2.351 (2) | C14—C15 | 1.375 (4) |
| Cl—O3 | 1.415 (3) | C14—H14 | 0.9500 |
| Cl—O4 | 1.416 (3) | C15—C16 | 1.408 (4) |
| Cl—O6 | 1.436 (2) | C15—H15 | 0.9500 |
| Cl—O5 | 1.442 (3) | C16—C17 | 1.385 (4) |
| O1—C28 | 1.2697 (10) | C16—H16 | 0.9500 |
| O2—C28 | 1.2403 (10) | C17—C18 | 1.390 (4) |
| O1′—C28 | 1.2697 (10) | C17—H17 | 0.9500 |
| O2′—C28 | 1.2401 (10) | C19—C20 | 1.497 (4) |
| O7—C33 | 1.229 (5) | C19—H19A | 0.9900 |
| O8—C34 | 1.391 (4) | C19—H19B | 0.9900 |
| O8—H8O | 0.8400 | C21—H21A | 0.9800 |
| N1—C2 | 1.321 (3) | C21—H21B | 0.9800 |
| N1—C9 | 1.395 (3) | C21—H21C | 0.9800 |
| N2—C2 | 1.350 (3) | C22—C23 | 1.389 (4) |
| N2—C4 | 1.384 (3) | C22—C27 | 1.398 (4) |
| N2—C3 | 1.462 (3) | C23—C24 | 1.370 (5) |
| N3—C11 | 1.325 (3) | C23—H23 | 0.9500 |
| N3—C18 | 1.402 (3) | C24—C25 | 1.390 (5) |
| N4—C11 | 1.344 (3) | C24—H24 | 0.9500 |
| N4—C13 | 1.387 (4) | C25—C26 | 1.381 (4) |
| N4—C12 | 1.462 (3) | C25—H25 | 0.9500 |
| N5—C20 | 1.327 (3) | C26—C27 | 1.385 (4) |
| N5—C27 | 1.400 (3) | C26—H26 | 0.9500 |
| N6—C20 | 1.345 (3) | C28—C29′ | 1.27 (4) |
| N6—C22 | 1.382 (4) | C28—C29 | 1.488 (4) |
| N6—C21 | 1.466 (4) | C29—C30 | 1.297 (5) |
| N7—C10 | 1.470 (3) | C29—H29 | 0.9500 |
| N7—C19 | 1.470 (3) | C29′—C30 | 1.31 (4) |
| N7—C1 | 1.476 (3) | C29′—H29′ | 0.9500 |
| N10—C33 | 1.318 (5) | C30—H30A | 0.9500 |
| N10—C32 | 1.443 (5) | C30—H30B | 0.9500 |
| N10—C31 | 1.461 (6) | C31—H31A | 0.9800 |
| C1—C2 | 1.486 (3) | C31—H31B | 0.9800 |
| C1—H1A | 0.9900 | C31—H31C | 0.9800 |
| C1—H1B | 0.9900 | C32—H32A | 0.9800 |
| C3—H3A | 0.9800 | C32—H32B | 0.9800 |
| C3—H3B | 0.9800 | C32—H32C | 0.9800 |

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|---|---|---|---|
| C3—H3C | 0.9800 | C33—H33 | 0.9500 |
| C4—C5 | 1.395 (4) | C34—H34A | 0.9800 |
| C4—C9 | 1.401 (4) | C34—H34B | 0.9800 |
| C5—C6 | 1.372 (4) | C34—H34C | 0.9800 |
| C5—H5 | 0.9500 | C35—O9 | 1.441 (3) |
| C6—C7 | 1.403 (4) | C35—H35A | 0.9800 |
| C6—H6 | 0.9500 | C35—H35B | 0.9800 |
| C7—C8 | 1.387 (4) | C35—H35C | 0.9800 |
| C7—H7 | 0.9500 | O9—H9O | 0.8400 |
| C8—C9 | 1.391 (4) | O9′—C35′ | 1.439 (3) |
| C8—H8 | 0.9500 | O9′—H9O′ | 0.8400 |
| C10—C11 | 1.484 (4) | C35′—H35D | 0.9800 |
| C10—H10A | 0.9900 | C35′—H35E | 0.9800 |
| C10—H10B | 0.9900 | C35′—H35F | 0.9800 |

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| O1′—Co—O1 | 34.4 (6) | C14—C15—H15 | 119.2 |
| O1′—Co—N1 | 123.9 (7) | C16—C15—H15 | 119.2 |
| O1—Co—N1 | 91.92 (8) | C17—C16—C15 | 121.6 (3) |
| O1′—Co—N3 | 101.8 (7) | C17—C16—H16 | 119.2 |
| O1—Co—N3 | 108.26 (9) | C15—C16—H16 | 119.2 |
| N1—Co—N3 | 114.07 (8) | C16—C17—C18 | 117.4 (3) |
| O1′—Co—N5 | 87.5 (5) | C16—C17—H17 | 121.3 |
| O1—Co—N5 | 113.55 (9) | C18—C17—H17 | 121.3 |
| N1—Co—N5 | 112.69 (8) | C17—C18—N3 | 131.4 (2) |
| N3—Co—N5 | 114.27 (8) | C17—C18—C13 | 120.3 (2) |
| O1′—Co—N7 | 158.7 (6) | N3—C18—C13 | 108.3 (2) |
| O1—Co—N7 | 166.76 (8) | N7—C19—C20 | 106.8 (2) |
| N1—Co—N7 | 75.20 (8) | N7—C19—H19A | 110.4 |
| N3—Co—N7 | 75.19 (8) | C20—C19—H19A | 110.4 |
| N5—Co—N7 | 75.09 (8) | N7—C19—H19B | 110.4 |
| O3—Cl—O4 | 110.2 (2) | C20—C19—H19B | 110.4 |
| O3—Cl—O6 | 109.93 (17) | H19A—C19—H19B | 108.6 |
| O4—Cl—O6 | 111.49 (18) | N5—C20—N6 | 112.5 (2) |
| O3—Cl—O5 | 108.3 (2) | N5—C20—C19 | 121.7 (2) |
| O4—Cl—O5 | 108.69 (18) | N6—C20—C19 | 125.7 (2) |
| O6—Cl—O5 | 108.10 (14) | N6—C21—H21A | 109.5 |
| C28—O1—Co | 121.23 (17) | N6—C21—H21B | 109.5 |
| C28—O1′—Co | 139.7 (14) | H21A—C21—H21B | 109.5 |
| C34—O8—H8O | 109.5 | N6—C21—H21C | 109.5 |
| C2—N1—C9 | 105.8 (2) | H21A—C21—H21C | 109.5 |
| C2—N1—Co | 117.75 (17) | H21B—C21—H21C | 109.5 |
| C9—N1—Co | 136.15 (17) | N6—C22—C23 | 131.5 (3) |
| C2—N2—C4 | 107.0 (2) | N6—C22—C27 | 106.3 (2) |
| C2—N2—C3 | 127.1 (2) | C23—C22—C27 | 122.1 (3) |
| C4—N2—C3 | 125.9 (2) | C24—C23—C22 | 116.4 (3) |
| C11—N3—C18 | 105.5 (2) | C24—C23—H23 | 121.8 |
| C11—N3—Co | 117.02 (16) | C22—C23—H23 | 121.8 |
| C18—N3—Co | 136.71 (17) | C23—C24—C25 | 122.1 (3) |

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| C11—N4—C13 | 107.2 (2) | C23—C24—H24 | 118.9 |
| C11—N4—C12 | 126.3 (2) | C25—C24—H24 | 118.9 |
| C13—N4—C12 | 126.5 (2) | C26—C25—C24 | 121.5 (3) |
| C20—N5—C27 | 105.8 (2) | C26—C25—H25 | 119.3 |
| C20—N5—Co | 117.45 (17) | C24—C25—H25 | 119.3 |
| C27—N5—Co | 136.56 (18) | C25—C26—C27 | 117.3 (3) |
| C20—N6—C22 | 107.2 (2) | C25—C26—H26 | 121.3 |
| C20—N6—C21 | 127.4 (2) | C27—C26—H26 | 121.3 |
| C22—N6—C21 | 125.3 (2) | C26—C27—C22 | 120.4 (3) |
| C10—N7—C19 | 111.3 (2) | C26—C27—N5 | 131.4 (3) |
| C10—N7—C1 | 112.0 (2) | C22—C27—N5 | 108.1 (2) |
| C19—N7—C1 | 112.4 (2) | O2′—C28—O2 | 144.7 (14) |
| C10—N7—Co | 107.01 (15) | O2′—C28—C29′ | 111 (3) |
| C19—N7—Co | 107.62 (15) | O2—C28—C29′ | 85 (3) |
| C1—N7—Co | 106.10 (15) | O2′—C28—O1′ | 103 (2) |
| C33—N10—C32 | 121.7 (3) | O2—C28—O1′ | 71.9 (11) |
| C33—N10—C31 | 121.1 (3) | C29′—C28—O1′ | 146 (3) |
| C32—N10—C31 | 117.2 (4) | O2′—C28—O1 | 54.9 (17) |
| N7—C1—C2 | 107.9 (2) | O2—C28—O1 | 123.8 (2) |
| N7—C1—H1A | 110.1 | C29′—C28—O1 | 148 (2) |
| C2—C1—H1A | 110.1 | O1′—C28—O1 | 52.9 (10) |
| N7—C1—H1B | 110.1 | O2′—C28—C29 | 74.2 (17) |
| C2—C1—H1B | 110.1 | O2—C28—C29 | 120.1 (2) |
| H1A—C1—H1B | 108.4 | C29′—C28—C29 | 37 (3) |
| N1—C2—N2 | 112.7 (2) | O1′—C28—C29 | 163.6 (11) |
| N1—C2—C1 | 121.5 (2) | O1—C28—C29 | 116.1 (2) |
| N2—C2—C1 | 125.7 (2) | C30—C29—C28 | 123.5 (4) |
| N2—C3—H3A | 109.5 | C30—C29—H29 | 118.2 |
| N2—C3—H3B | 109.5 | C28—C29—H29 | 118.2 |
| H3A—C3—H3B | 109.5 | C28—C29′—C30 | 145 (4) |
| N2—C3—H3C | 109.5 | C28—C29′—H29′ | 107.4 |
| H3A—C3—H3C | 109.5 | C30—C29′—H29′ | 107.4 |
| H3B—C3—H3C | 109.5 | C29—C30—C29′ | 41 (3) |
| N2—C4—C5 | 132.2 (3) | C29—C30—H30A | 120.0 |
| N2—C4—C9 | 106.0 (2) | C29′—C30—H30A | 81.9 |
| C5—C4—C9 | 121.8 (3) | C29—C30—H30B | 120.0 |
| C6—C5—C4 | 116.9 (3) | C29′—C30—H30B | 153.8 |
| C6—C5—H5 | 121.6 | H30A—C30—H30B | 120.0 |
| C4—C5—H5 | 121.6 | N10—C31—H31A | 109.5 |
| C5—C6—C7 | 122.0 (3) | N10—C31—H31B | 109.5 |
| C5—C6—H6 | 119.0 | H31A—C31—H31B | 109.5 |
| C7—C6—H6 | 119.0 | N10—C31—H31C | 109.5 |
| C8—C7—C6 | 121.1 (3) | H31A—C31—H31C | 109.5 |
| C8—C7—H7 | 119.5 | H31B—C31—H31C | 109.5 |
| C6—C7—H7 | 119.5 | N10—C32—H32A | 109.5 |
| C7—C8—C9 | 117.5 (3) | N10—C32—H32B | 109.5 |
| C7—C8—H8 | 121.3 | H32A—C32—H32B | 109.5 |
| C9—C8—H8 | 121.3 | N10—C32—H32C | 109.5 |

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| C8—C9—N1 | 130.8 (2) | H32A—C32—H32C | 109.5 |
| C8—C9—C4 | 120.8 (2) | H32B—C32—H32C | 109.5 |
| N1—C9—C4 | 108.4 (2) | O7—C33—N10 | 125.8 (4) |
| N7—C10—C11 | 108.0 (2) | O7—C33—H33 | 117.1 |
| N7—C10—H10A | 110.1 | N10—C33—H33 | 117.1 |
| C11—C10—H10A | 110.1 | O8—C34—H34A | 109.5 |
| N7—C10—H10B | 110.1 | O8—C34—H34B | 109.5 |
| C11—C10—H10B | 110.1 | H34A—C34—H34B | 109.5 |
| H10A—C10—H10B | 108.4 | O8—C34—H34C | 109.5 |
| N3—C11—N4 | 113.1 (2) | H34A—C34—H34C | 109.5 |
| N3—C11—C10 | 122.5 (2) | H34B—C34—H34C | 109.5 |
| N4—C11—C10 | 124.3 (2) | O9—C35—H35A | 109.5 |
| N4—C12—H12A | 109.5 | O9—C35—H35B | 109.5 |
| N4—C12—H12B | 109.5 | H35A—C35—H35B | 109.5 |
| H12A—C12—H12B | 109.5 | O9—C35—H35C | 109.5 |
| N4—C12—H12C | 109.5 | H35A—C35—H35C | 109.5 |
| H12A—C12—H12C | 109.5 | H35B—C35—H35C | 109.5 |
| H12B—C12—H12C | 109.5 | C35—O9—H9O | 109.5 |
| N4—C13—C14 | 131.7 (2) | C35′—O9′—H9O′ | 109.5 |
| N4—C13—C18 | 105.9 (2) | O9′—C35′—H35D | 109.5 |
| C14—C13—C18 | 122.4 (3) | O9′—C35′—H35E | 109.5 |
| C15—C14—C13 | 116.7 (3) | H35D—C35′—H35E | 109.5 |
| C15—C14—H14 | 121.7 | O9′—C35′—H35F | 109.5 |
| C13—C14—H14 | 121.7 | H35D—C35′—H35F | 109.5 |
| C14—C15—C16 | 121.6 (2) | H35E—C35′—H35F | 109.5 |

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| O1′—Co—O1—C28 | 24.9 (11) | C1—N7—C10—C11 | 84.9 (2) |
| N1—Co—O1—C28 | −175.5 (2) | Co—N7—C10—C11 | −31.0 (2) |
| N3—Co—O1—C28 | −59.3 (2) | C18—N3—C11—N4 | 1.0 (3) |
| N5—Co—O1—C28 | 68.7 (2) | Co—N3—C11—N4 | −170.57 (16) |
| N7—Co—O1—C28 | −162.4 (3) | C18—N3—C11—C10 | 178.6 (2) |
| O1—Co—O1′—C28 | −33.8 (17) | Co—N3—C11—C10 | 7.1 (3) |
| N1—Co—O1′—C28 | −59 (3) | C13—N4—C11—N3 | −1.2 (3) |
| N3—Co—O1′—C28 | 71 (3) | C12—N4—C11—N3 | −178.7 (2) |
| N5—Co—O1′—C28 | −174 (2) | C13—N4—C11—C10 | −178.8 (2) |
| N7—Co—O1′—C28 | 150.8 (11) | C12—N4—C11—C10 | 3.7 (4) |
| O1′—Co—N1—C2 | 173.3 (7) | N7—C10—C11—N3 | 19.1 (3) |
| O1—Co—N1—C2 | 159.57 (19) | N7—C10—C11—N4 | −163.5 (2) |
| N3—Co—N1—C2 | 48.6 (2) | C11—N4—C13—C14 | 179.7 (3) |
| N5—Co—N1—C2 | −83.86 (19) | C12—N4—C13—C14 | −2.8 (4) |
| N7—Co—N1—C2 | −17.37 (17) | C11—N4—C13—C18 | 0.8 (3) |
| O1′—Co—N1—C9 | 0.4 (7) | C12—N4—C13—C18 | 178.3 (2) |
| O1—Co—N1—C9 | −13.3 (2) | N4—C13—C14—C15 | −179.9 (3) |
| N3—Co—N1—C9 | −124.3 (2) | C18—C13—C14—C15 | −1.2 (4) |
| N5—Co—N1—C9 | 103.3 (2) | C13—C14—C15—C16 | 0.6 (4) |
| N7—Co—N1—C9 | 169.8 (2) | C14—C15—C16—C17 | 0.3 (4) |
| O1′—Co—N3—C11 | 139.2 (6) | C15—C16—C17—C18 | −0.6 (4) |
| O1—Co—N3—C11 | 174.25 (17) | C16—C17—C18—N3 | −179.8 (3) |

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| N1—Co—N3—C11 | −85.03 (19) | C16—C17—C18—C13 | 0.0 (4) |
| N5—Co—N3—C11 | 46.6 (2) | C11—N3—C18—C17 | 179.4 (3) |
| N7—Co—N3—C11 | −19.08 (17) | Co—N3—C18—C17 | −11.6 (4) |
| O1′—Co—N3—C18 | −28.9 (6) | C11—N3—C18—C13 | −0.4 (3) |
| O1—Co—N3—C18 | 6.1 (3) | Co—N3—C18—C13 | 168.59 (18) |
| N1—Co—N3—C18 | 106.8 (2) | N4—C13—C18—C17 | 179.9 (2) |
| N5—Co—N3—C18 | −121.5 (2) | C14—C13—C18—C17 | 0.9 (4) |
| N7—Co—N3—C18 | 172.8 (2) | N4—C13—C18—N3 | −0.2 (3) |
| O1′—Co—N5—C20 | 179.8 (8) | C14—C13—C18—N3 | −179.3 (2) |
| O1—Co—N5—C20 | 156.76 (18) | C10—N7—C19—C20 | 82.3 (2) |
| N1—Co—N5—C20 | 53.9 (2) | C1—N7—C19—C20 | −151.1 (2) |
| N3—Co—N5—C20 | −78.4 (2) | Co—N7—C19—C20 | −34.6 (2) |
| N7—Co—N5—C20 | −12.61 (18) | C27—N5—C20—N6 | 0.0 (3) |
| O1′—Co—N5—C27 | −6.6 (8) | Co—N5—C20—N6 | 175.43 (16) |
| O1—Co—N5—C27 | −29.6 (3) | C27—N5—C20—C19 | −179.9 (2) |
| N1—Co—N5—C27 | −132.4 (2) | Co—N5—C20—C19 | −4.5 (3) |
| N3—Co—N5—C27 | 95.2 (2) | C22—N6—C20—N5 | −0.9 (3) |
| N7—Co—N5—C27 | 161.0 (3) | C21—N6—C20—N5 | 178.5 (2) |
| O1′—Co—N7—C10 | −56.6 (18) | C22—N6—C20—C19 | 179.0 (2) |
| O1—Co—N7—C10 | 134.8 (3) | C21—N6—C20—C19 | −1.5 (4) |
| N1—Co—N7—C10 | 148.29 (17) | N7—C19—C20—N5 | 28.7 (3) |
| N3—Co—N7—C10 | 27.88 (15) | N7—C19—C20—N6 | −151.2 (2) |
| N5—Co—N7—C10 | −92.81 (16) | C20—N6—C22—C23 | −177.3 (3) |
| O1′—Co—N7—C19 | 63.2 (18) | C21—N6—C22—C23 | 3.3 (5) |
| O1—Co—N7—C19 | −105.4 (4) | C20—N6—C22—C27 | 1.4 (3) |
| N1—Co—N7—C19 | −91.96 (16) | C21—N6—C22—C27 | −178.0 (2) |
| N3—Co—N7—C19 | 147.62 (17) | N6—C22—C23—C24 | −179.1 (3) |
| N5—Co—N7—C19 | 26.94 (16) | C27—C22—C23—C24 | 2.3 (4) |
| O1′—Co—N7—C1 | −176.3 (18) | C22—C23—C24—C25 | −0.1 (5) |
| O1—Co—N7—C1 | 15.1 (4) | C23—C24—C25—C26 | −1.7 (5) |
| N1—Co—N7—C1 | 28.55 (15) | C24—C25—C26—C27 | 1.1 (4) |
| N3—Co—N7—C1 | −91.87 (16) | C25—C26—C27—C22 | 1.1 (4) |
| N5—Co—N7—C1 | 147.44 (16) | C25—C26—C27—N5 | −179.3 (3) |
| C10—N7—C1—C2 | −150.4 (2) | N6—C22—C27—C26 | 178.2 (2) |
| C19—N7—C1—C2 | 83.4 (3) | C23—C22—C27—C26 | −2.9 (4) |
| Co—N7—C1—C2 | −34.0 (2) | N6—C22—C27—N5 | −1.5 (3) |
| C9—N1—C2—N2 | −0.4 (3) | C23—C22—C27—N5 | 177.4 (2) |
| Co—N1—C2—N2 | −175.23 (16) | C20—N5—C27—C26 | −178.7 (3) |
| C9—N1—C2—C1 | 177.3 (2) | Co—N5—C27—C26 | 7.2 (5) |
| Co—N1—C2—C1 | 2.5 (3) | C20—N5—C27—C22 | 0.9 (3) |
| C4—N2—C2—N1 | 0.2 (3) | Co—N5—C27—C22 | −173.20 (19) |
| C3—N2—C2—N1 | 177.5 (2) | Co—O1′—C28—O2′ | 13 (3) |
| C4—N2—C2—C1 | −177.4 (2) | Co—O1′—C28—O2 | −131 (3) |
| C3—N2—C2—C1 | −0.1 (4) | Co—O1′—C28—C29′ | −180 (4) |
| N7—C1—C2—N1 | 24.3 (3) | Co—O1′—C28—O1 | 38.1 (18) |
| N7—C1—C2—N2 | −158.3 (2) | Co—O1′—C28—C29 | 90 (4) |
| C2—N2—C4—C5 | −179.8 (3) | Co—O1—C28—O2′ | 125.3 (17) |
| C3—N2—C4—C5 | 2.7 (4) | Co—O1—C28—O2 | −11.5 (4) |

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| C2—N2—C4—C9 | 0.2 (3) | Co—O1—C28—C29′ | −163 (4) |
| C3—N2—C4—C9 | −177.3 (2) | Co—O1—C28—O1′ | −24.6 (12) |
| N2—C4—C5—C6 | 179.7 (3) | Co—O1—C28—C29 | 169.7 (2) |
| C9—C4—C5—C6 | −0.3 (4) | O2′—C28—C29—C30 | −140.1 (15) |
| C4—C5—C6—C7 | 0.5 (4) | O2—C28—C29—C30 | 4.6 (5) |
| C5—C6—C7—C8 | −0.6 (5) | C29′—C28—C29—C30 | 26 (3) |
| C6—C7—C8—C9 | 0.4 (4) | O1′—C28—C29—C30 | 139 (3) |
| C7—C8—C9—N1 | −179.5 (3) | O1—C28—C29—C30 | −176.6 (3) |
| C7—C8—C9—C4 | −0.2 (4) | O2′—C28—C29′—C30 | −26 (8) |
| C2—N1—C9—C8 | 179.8 (3) | O2—C28—C29′—C30 | 121 (7) |
| Co—N1—C9—C8 | −6.8 (4) | O1′—C28—C29′—C30 | 168 (5) |
| C2—N1—C9—C4 | 0.5 (3) | O1—C28—C29′—C30 | −82 (7) |
| Co—N1—C9—C4 | 173.88 (18) | C29—C28—C29′—C30 | −40 (6) |
| N2—C4—C9—C8 | −179.8 (2) | C28—C29—C30—C29′ | −24 (2) |
| C5—C4—C9—C8 | 0.2 (4) | C28—C29′—C30—C29 | 43 (6) |
| N2—C4—C9—N1 | −0.4 (3) | C32—N10—C33—O7 | −2.0 (6) |
| C5—C4—C9—N1 | 179.6 (2) | C31—N10—C33—O7 | 175.7 (5) |
| C19—N7—C10—C11 | −148.3 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O8—H8*O*···O7$^{i}$ | 0.84 | 1.94 | 2.765 (4) | 169 |

Symmetry code: (i) −*x*+2, −*y*+2, −*z*+1.