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# Bis{2-bromo-4-chloro-6-[(*E*)-(2,6-dimethylphenyl)iminomethyl]phenolato- $\kappa^2N,O$ }cobalt(II)

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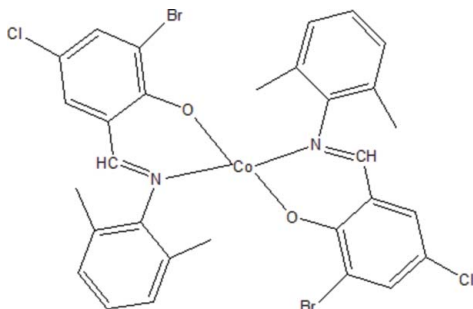
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Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.044;  $wR$  factor = 0.119; data-to-parameter ratio = 21.7.

In the title complex,  $[Co(C_{15}H_{12}BrClNO)_2]$ , the  $Co^{II}$  ion is coordinated by two *N,O*-bidentate 2-bromo-4-chloro-6-[(*E*)-(2,6-dimethylphenyl)iminomethyl]phenolate ligands, generating a squashed  $CoN_2O_2$  tetrahedral coordination geometry. The dihedral angles between the aromatic rings in the ligands are 82.60 (14) and 71.79 (14)°. The complex has approximate local noncrystallographic twofold symmetry. In the crystal, weak aromatic  $\pi-\pi$  stacking is observed [centroid-centroid separation = 3.6434 (18) Å].

## Related literature

For background to Schiff bases, see: Billson *et al.* (2000); Carlton *et al.* (1995); Feng *et al.* (2008); Liu *et al.* (2009).



## Experimental

### Crystal data

 $[Co(C_{15}H_{12}BrClNO)_2]$  $M_r = 734.16$ 

Monoclinic,  $P2_1/c$   
 $a = 11.608$  (2) Å  
 $b = 24.157$  (4) Å  
 $c = 11.354$  (2) Å  
 $\beta = 114.380$  (2)°  
 $V = 2899.8$  (9) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.56$  mm<sup>-1</sup>  
 $T = 153$  K  
 $0.49 \times 0.27 \times 0.12$  mm

### Data collection

Rigaku AFC10/Saturn724+ diffractometer  
 Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)  
 $T_{min} = 0.274$ ,  $T_{max} = 0.683$

32947 measured reflections  
 7718 independent reflections  
 6813 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.047$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.119$   
 $S = 1.00$   
 7718 reflections

356 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 0.54$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.63$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Co1—O2	1.9006 (18)	Co1—N2	1.983 (2)
Co1—O1	1.9144 (18)	Co1—N1	2.000 (2)

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: HB7032).

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## supporting information

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## Bis{2-bromo-4-chloro-6-[(*E*)-(2,6-dimethylphenyl)iminomethyl]phenolato- $\kappa^2N,O$ }cobalt(II)

Gang Zhu and Bao-Juan Jiao

### S1. Comment

Schiff bases possess strong coordination function and may act as bi-, tri-, and poly-dentate ligands to yield plenty of mono-, bi-, tri-, and poly-nuclear Schiff-base complexes, so the design of metal-organic coordination polymers is of current interest in the fields of supramolecular chemistry and crystal engineering because of their potential applications as functional materials (Feng, *et al.*, 2008; Liu, *et al.*, 2009). Meanwhile, Schiff bases and their metal complexes exhibit biological activity as antibiotics, antiviral and antitumour agents because of their specific structures (Billson, *et al.*, 2000; Carlton, *et al.*, 1995). Thus, it is quite important to have a good understanding of the structure of such metal complexes.

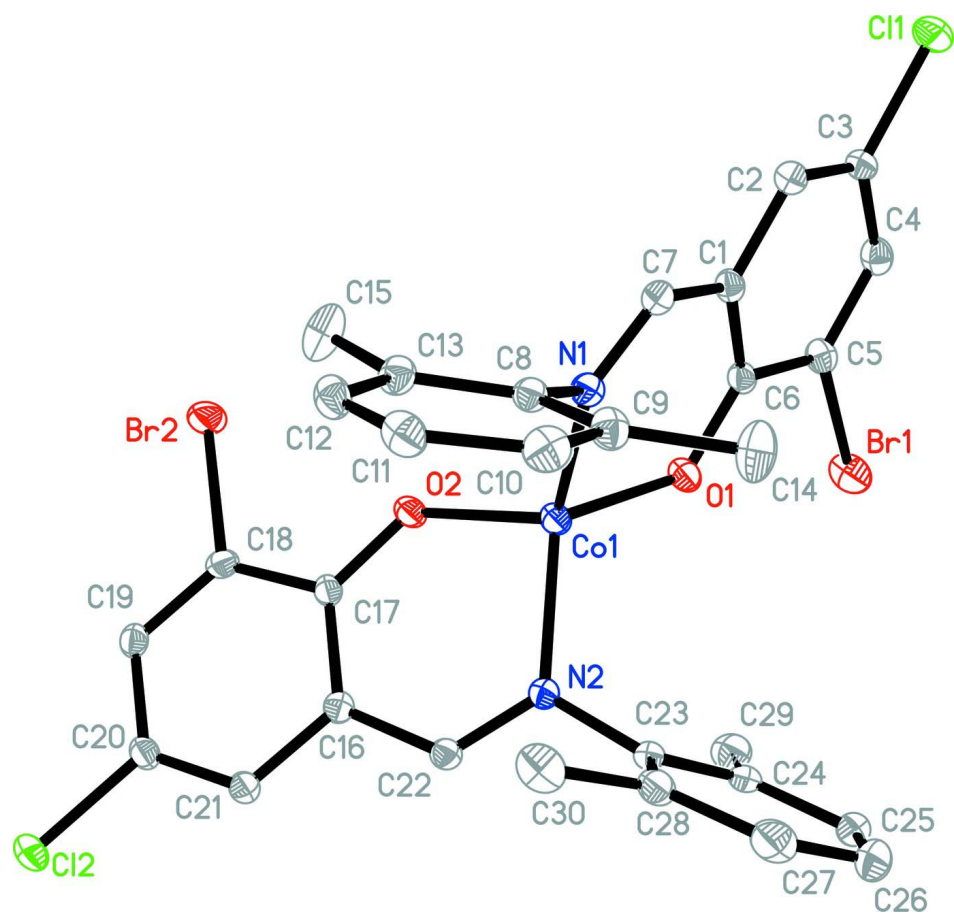
In this paper, we report synthesis and crystal structure of a new cobalt(II) complex, bis[2-((*E*)-(2,6-dimethylphenyl-imino) methyl)-6-bromo-4-chlorophenol]cobalt(II). The structure of the complex had been established accurately from the X-ray single-crystal diffraction study. The Co(II) ion in the monomeric unit seems to reside in a distorted tetrahedral environment and bonds to two oxygen atoms and two nitrogen atoms from two Schiff bases.

A thermal ellipsoid drawing and crystal packing structure of the title complex are shown in Figure 1 and Figure 2. The Co(C<sub>15</sub>H<sub>12</sub>BrClNO)<sub>2</sub> motif is asymmetrical with Co—N and Co—O bonds, the corresponding distances are  $d(\text{Co—N1}) = 2.000$  (2),  $d(\text{Co—O1}) = 1.9144$  (18),  $d(\text{Co—N2}) = 1.983$  (2),  $d(\text{Co—O2}) = 1.9006$  (2) Å. The cobalt atom is in a distorted tetrahedral environment, where the values of *trans* bond angles also indicate the coordination environment with O(2)—Co(1)—N(1), O(2)—Co(1)—N(2) and O(2)—Co(1)—O(1) angles of 116.97 (9), 94.94 (8) and 113.77 (8) °, respectively.

In the crystal structure of the complex the atoms of the phenyl ring plane A (C(1) C(2) C(3) C(4) C(5) C(6)) and the chelate ring formed by the same ligand plane B ((O(1)/Co(1)/N(1)/C(7)/C(1)/C(6)) are nearly coplanar with a dihedral angle of 8.09 (10) °. Because of the conjugation effects through the imino double bond N(1)=C(7), the phenyl ring A and the phenyl ring C (C(8) C(9) C(10) C(11) C(12) C(13)) joined by the N(1)=C(7) bond, are non-coplanar (with the dihedral angle 74.55 (7) °, decreasing the steric effects between the two rings. If the two chelate planes, planes B and D((N(2)/Co(1)/O(2)/C(17)/C(16)/C(22)), are compared the dihedral angle is 87.19 (6) °, nearly perpendicular.

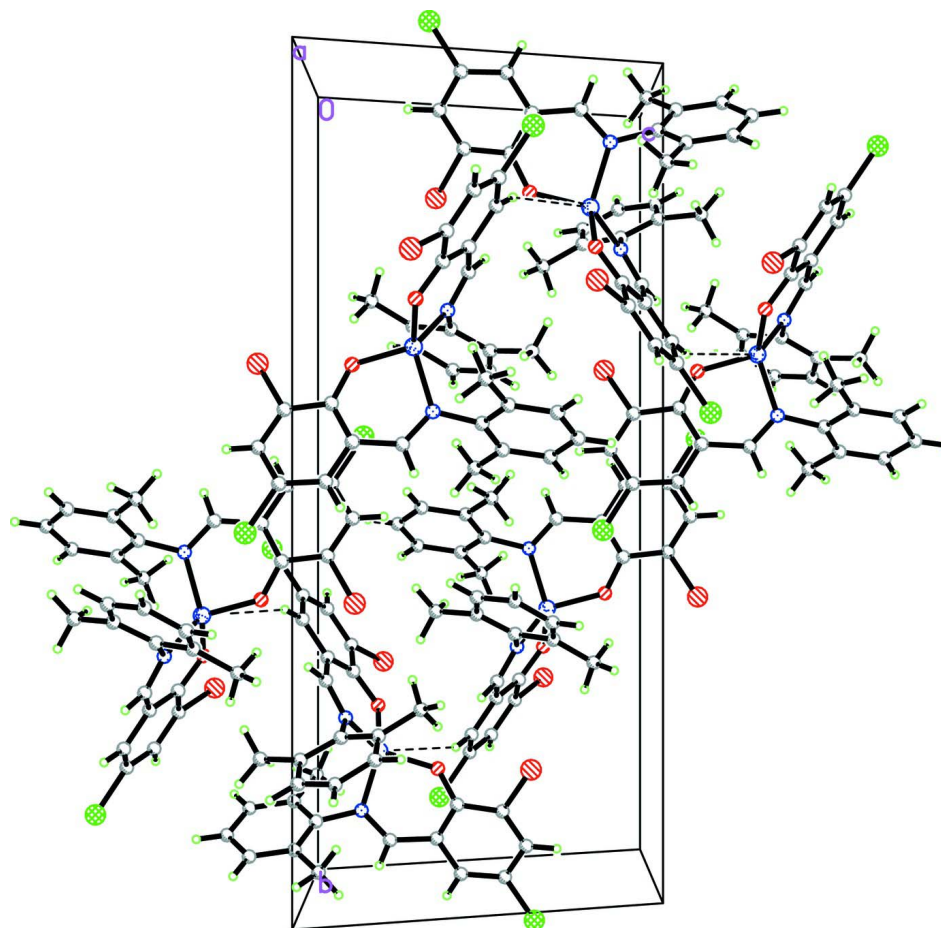
### S2. Experimental

3-Bromo-5-chlorosalicylaldehyde (0.2 mmol, 47.2 mg) and 2,6-Dimethylaniline (0.2 mmol, 24.2 mg) were dissolved in EtOH (15 mL). The mixture was stirred for 30 min at room temperature to give an orange solution. To the resulting orange solution was added Co(CH<sub>3</sub>COO)<sub>2</sub> (0.1 mmol, 17.7 mg). Then a clear brown solution was obtained. The title complex were obtained from the solution after 4 d in the form of red chunks. The product was filtered, washed with EtOH, and dried over anhydrous CaCl<sub>2</sub> *in vacuo* overnight. Yield: 70%. Anal. Calcd. (%) for C<sub>30</sub>H<sub>24</sub>CoN<sub>2</sub>O<sub>2</sub>Cl<sub>2</sub>Br<sub>2</sub>: C, 49.08; H, 3.29; N, 3.82. Found (%): C, 49.13; H, 3.43; N, 3.70.



**Figure 1**

The structure of the title complex in 30% probability ellipsoids. H atoms are deleted for clarity.

**Figure 2**

The crystal packing of the title complex, viewed along the *a* axis.

**Bis{2-bromo-4-chloro-6-[(*E*)-(2,6-dimethylphenyl)iminomethyl]phenolato- $\kappa^2N,O$ }cobalt(II)**

*Crystal data*

[Co(C<sub>15</sub>H<sub>12</sub>BrClNO)<sub>2</sub>]

*M<sub>r</sub>* = 734.16

Monoclinic, *P*2<sub>1</sub>/*c*

*a* = 11.608 (2) Å

*b* = 24.157 (4) Å

*c* = 11.354 (2) Å

$\beta$  = 114.380 (2)°

*V* = 2899.8 (9) Å<sup>3</sup>

*Z* = 4

*F*(000) = 1460

*D<sub>x</sub>* = 1.682 Mg m<sup>-3</sup>

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

Cell parameters from 10097 reflections

$\theta$  = 2.1–29.1°

$\mu$  = 3.56 mm<sup>-1</sup>

*T* = 153 K

Chunk, red

0.49 × 0.27 × 0.12 mm

*Data collection*

Rigaku AFC10/Saturn724+  
diffractometer

Radiation source: Rotating Anode

Graphite monochromator

Detector resolution: 28.5714 pixels mm<sup>-1</sup>

phi and  $\omega$  scans

Absorption correction: multi-scan  
(*CrystalClear*; Rigaku, 2008)

*T<sub>min</sub>* = 0.274, *T<sub>max</sub>* = 0.683

32947 measured reflections

7718 independent reflections

6813 reflections with *I* > 2 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.047

$\theta_{\max} = 29.1^\circ$ ,  $\theta_{\min} = 2.3^\circ$   
 $h = -15 \rightarrow 15$

$k = -33 \rightarrow 32$   
 $l = -15 \rightarrow 15$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.119$   
 $S = 1.00$   
 7718 reflections  
 356 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 0.516P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.54 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.63 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.26654 (3)	0.662257 (15)	0.69368 (3)	0.02274 (10)
Br1	0.57530 (3)	0.644847 (13)	1.13829 (3)	0.03965 (10)
Br2	-0.09274 (3)	0.764024 (13)	0.69082 (3)	0.04195 (10)
Cl1	0.36329 (7)	0.44165 (3)	1.15246 (7)	0.03762 (18)
Cl2	-0.01848 (7)	0.91557 (3)	0.36421 (7)	0.03602 (17)
O1	0.37754 (18)	0.64192 (7)	0.86650 (17)	0.0264 (4)
O2	0.14215 (17)	0.71526 (7)	0.68464 (18)	0.0272 (4)
N1	0.2067 (2)	0.58493 (9)	0.6390 (2)	0.0234 (5)
N2	0.34280 (19)	0.70873 (9)	0.60062 (19)	0.0208 (4)
C1	0.2975 (2)	0.54925 (11)	0.8618 (2)	0.0231 (5)
C2	0.2949 (2)	0.50225 (11)	0.9335 (3)	0.0270 (6)
H2	0.2416	0.4720	0.8913	0.032*
C3	0.3687 (2)	0.49968 (11)	1.0639 (3)	0.0277 (6)
C4	0.4516 (3)	0.54284 (12)	1.1261 (3)	0.0287 (6)
H4	0.5049	0.5406	1.2158	0.034*
C5	0.4548 (3)	0.58833 (11)	1.0562 (2)	0.0259 (6)
C6	0.3753 (2)	0.59526 (10)	0.9230 (2)	0.0225 (5)
C7	0.2230 (2)	0.54617 (11)	0.7227 (3)	0.0254 (5)
H7	0.1819	0.5119	0.6900	0.030*
C8	0.1440 (2)	0.57063 (11)	0.5034 (2)	0.0239 (5)
C9	0.2103 (3)	0.53997 (11)	0.4467 (3)	0.0291 (6)
C10	0.1533 (3)	0.53156 (12)	0.3131 (3)	0.0326 (6)
H10	0.1964	0.5108	0.2726	0.039*

C11	0.0347 (3)	0.55301 (12)	0.2391 (3)	0.0320 (6)
H11	-0.0025	0.5475	0.1481	0.038*
C12	-0.0294 (3)	0.58239 (11)	0.2975 (3)	0.0297 (6)
H12	-0.1105	0.5971	0.2456	0.036*
C13	0.0222 (3)	0.59107 (12)	0.4314 (3)	0.0280 (6)
C14	0.3415 (3)	0.51866 (15)	0.5239 (3)	0.0443 (8)
H14A	0.3946	0.5487	0.5766	0.053*
H14B	0.3773	0.5047	0.4651	0.053*
H14C	0.3382	0.4886	0.5804	0.053*
C15	-0.0532 (3)	0.62008 (16)	0.4928 (3)	0.0455 (8)
H15A	-0.0562	0.5971	0.5626	0.055*
H15B	-0.1394	0.6265	0.4277	0.055*
H15C	-0.0134	0.6556	0.5282	0.055*
C16	0.1773 (2)	0.77951 (10)	0.5396 (2)	0.0210 (5)
C17	0.1093 (2)	0.75899 (10)	0.6102 (2)	0.0208 (5)
C18	0.0010 (2)	0.78977 (11)	0.5987 (3)	0.0247 (5)
C19	-0.0383 (2)	0.83669 (11)	0.5250 (3)	0.0244 (5)
H19	-0.1116	0.8560	0.5198	0.029*
C20	0.0307 (2)	0.85564 (11)	0.4578 (3)	0.0250 (5)
C21	0.1359 (2)	0.82777 (10)	0.4642 (2)	0.0231 (5)
H21	0.1815	0.8412	0.4173	0.028*
C22	0.2909 (2)	0.75423 (11)	0.5415 (2)	0.0221 (5)
H22	0.3315	0.7727	0.4952	0.027*
C23	0.4569 (2)	0.68953 (11)	0.5936 (2)	0.0234 (5)
C24	0.5715 (2)	0.69448 (11)	0.7039 (3)	0.0269 (6)
C25	0.6783 (3)	0.67082 (13)	0.6988 (3)	0.0376 (7)
H25	0.7568	0.6735	0.7721	0.045*
C26	0.6736 (3)	0.64344 (14)	0.5902 (4)	0.0452 (9)
H26	0.7476	0.6267	0.5900	0.054*
C27	0.5609 (3)	0.64060 (13)	0.4820 (3)	0.0405 (8)
H27	0.5586	0.6225	0.4067	0.049*
C28	0.4499 (3)	0.66366 (12)	0.4805 (3)	0.0288 (6)
C29	0.5791 (3)	0.72459 (13)	0.8230 (3)	0.0357 (7)
H29A	0.5418	0.7016	0.8693	0.043*
H29B	0.5325	0.7596	0.7977	0.043*
H29C	0.6678	0.7322	0.8794	0.043*
C30	0.3284 (3)	0.66150 (13)	0.3601 (3)	0.0387 (7)
H30A	0.2577	0.6540	0.3838	0.046*
H30B	0.3336	0.6320	0.3032	0.046*
H30C	0.3148	0.6971	0.3148	0.046*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.02424 (18)	0.02062 (18)	0.02371 (19)	0.00174 (13)	0.01026 (15)	0.00289 (14)
Br1	0.04535 (19)	0.03466 (18)	0.02708 (17)	-0.00775 (13)	0.00302 (14)	-0.00110 (12)
Br2	0.03983 (18)	0.03857 (19)	0.0633 (2)	0.01156 (13)	0.03721 (17)	0.01945 (15)
Cl1	0.0409 (4)	0.0365 (4)	0.0354 (4)	0.0004 (3)	0.0157 (3)	0.0140 (3)

C12	0.0365 (4)	0.0288 (4)	0.0433 (4)	0.0091 (3)	0.0170 (3)	0.0161 (3)
O1	0.0289 (10)	0.0226 (10)	0.0251 (10)	0.0012 (7)	0.0084 (8)	0.0037 (8)
O2	0.0294 (10)	0.0232 (10)	0.0340 (10)	0.0063 (7)	0.0182 (8)	0.0091 (8)
N1	0.0228 (11)	0.0236 (11)	0.0233 (11)	-0.0004 (8)	0.0090 (9)	0.0003 (9)
N2	0.0201 (10)	0.0213 (11)	0.0214 (10)	0.0011 (8)	0.0091 (8)	0.0013 (8)
C1	0.0225 (12)	0.0230 (13)	0.0239 (13)	0.0043 (9)	0.0098 (10)	0.0019 (10)
C2	0.0248 (13)	0.0244 (14)	0.0317 (14)	0.0003 (10)	0.0115 (11)	0.0022 (11)
C3	0.0270 (13)	0.0263 (14)	0.0327 (15)	0.0033 (11)	0.0154 (12)	0.0093 (12)
C4	0.0299 (14)	0.0336 (15)	0.0229 (13)	0.0062 (11)	0.0113 (11)	0.0032 (11)
C5	0.0278 (13)	0.0241 (13)	0.0241 (13)	0.0021 (10)	0.0089 (11)	-0.0011 (11)
C6	0.0227 (12)	0.0237 (13)	0.0232 (13)	0.0044 (9)	0.0115 (10)	0.0038 (10)
C7	0.0213 (12)	0.0255 (13)	0.0287 (14)	0.0000 (10)	0.0096 (11)	0.0010 (11)
C8	0.0238 (12)	0.0243 (13)	0.0229 (13)	-0.0013 (10)	0.0091 (11)	0.0014 (10)
C9	0.0307 (14)	0.0244 (14)	0.0301 (15)	0.0008 (11)	0.0105 (12)	-0.0026 (11)
C10	0.0367 (16)	0.0277 (15)	0.0345 (16)	-0.0033 (12)	0.0160 (13)	-0.0094 (12)
C11	0.0378 (16)	0.0294 (15)	0.0218 (13)	-0.0041 (12)	0.0052 (12)	-0.0018 (11)
C12	0.0280 (14)	0.0270 (14)	0.0255 (14)	-0.0005 (11)	0.0022 (11)	-0.0002 (11)
C13	0.0259 (13)	0.0290 (15)	0.0270 (14)	-0.0015 (10)	0.0088 (11)	-0.0016 (11)
C14	0.0354 (17)	0.050 (2)	0.0422 (18)	0.0135 (14)	0.0113 (15)	-0.0085 (16)
C15	0.0268 (15)	0.065 (2)	0.0403 (18)	0.0040 (15)	0.0095 (14)	-0.0139 (17)
C16	0.0206 (12)	0.0188 (12)	0.0225 (12)	-0.0001 (9)	0.0078 (10)	-0.0020 (10)
C17	0.0200 (11)	0.0193 (12)	0.0210 (12)	0.0011 (9)	0.0063 (10)	0.0008 (10)
C18	0.0221 (12)	0.0251 (13)	0.0300 (14)	-0.0015 (10)	0.0139 (11)	0.0014 (11)
C19	0.0199 (12)	0.0235 (13)	0.0275 (14)	0.0032 (9)	0.0076 (10)	0.0008 (11)
C20	0.0257 (13)	0.0215 (13)	0.0248 (13)	0.0018 (10)	0.0075 (11)	0.0038 (10)
C21	0.0225 (12)	0.0228 (13)	0.0227 (13)	-0.0001 (10)	0.0080 (10)	0.0019 (10)
C22	0.0226 (12)	0.0227 (13)	0.0210 (12)	-0.0004 (9)	0.0090 (10)	0.0013 (10)
C23	0.0222 (12)	0.0239 (13)	0.0271 (13)	0.0026 (10)	0.0133 (11)	0.0075 (11)
C24	0.0239 (13)	0.0269 (14)	0.0310 (14)	-0.0002 (10)	0.0123 (11)	0.0118 (11)
C25	0.0246 (14)	0.0439 (18)	0.0441 (18)	0.0050 (12)	0.0140 (13)	0.0217 (15)
C26	0.0390 (18)	0.048 (2)	0.061 (2)	0.0186 (14)	0.0329 (17)	0.0210 (17)
C27	0.057 (2)	0.0370 (18)	0.0435 (18)	0.0131 (15)	0.0372 (17)	0.0081 (14)
C28	0.0340 (15)	0.0265 (14)	0.0303 (15)	0.0056 (11)	0.0178 (12)	0.0062 (11)
C29	0.0310 (15)	0.0383 (17)	0.0314 (16)	-0.0085 (12)	0.0066 (13)	0.0018 (13)
C30	0.0503 (19)	0.0364 (17)	0.0291 (16)	0.0005 (14)	0.0162 (14)	-0.0037 (13)

*Geometric parameters (Å, °)*

Co1—O2	1.9006 (18)	C13—C15	1.499 (4)
Co1—O1	1.9144 (18)	C14—H14A	0.9800
Co1—N2	1.983 (2)	C14—H14B	0.9800
Co1—N1	2.000 (2)	C14—H14C	0.9800
Br1—C5	1.901 (3)	C15—H15A	0.9800
Br2—C18	1.898 (3)	C15—H15B	0.9800
Cl1—C3	1.742 (3)	C15—H15C	0.9800
Cl2—C20	1.746 (3)	C16—C21	1.408 (3)
O1—C6	1.302 (3)	C16—C17	1.426 (4)
O2—C17	1.308 (3)	C16—C22	1.445 (3)

N1—C7	1.291 (3)	C17—C18	1.420 (3)
N1—C8	1.447 (3)	C18—C19	1.370 (4)
N2—C22	1.299 (3)	C19—C20	1.392 (4)
N2—C23	1.437 (3)	C19—H19	0.9500
C1—C2	1.405 (4)	C20—C21	1.370 (4)
C1—C6	1.420 (4)	C21—H21	0.9500
C1—C7	1.456 (4)	C22—H22	0.9500
C2—C3	1.372 (4)	C23—C28	1.400 (4)
C2—H2	0.9500	C23—C24	1.406 (4)
C3—C4	1.397 (4)	C24—C25	1.387 (4)
C4—C5	1.365 (4)	C24—C29	1.506 (4)
C4—H4	0.9500	C25—C26	1.381 (5)
C5—C6	1.420 (4)	C25—H25	0.9500
C7—H7	0.9500	C26—C27	1.378 (5)
C8—C13	1.399 (4)	C26—H26	0.9500
C8—C9	1.402 (4)	C27—C28	1.397 (4)
C9—C10	1.397 (4)	C27—H27	0.9500
C9—C14	1.500 (4)	C28—C30	1.506 (4)
C10—C11	1.383 (4)	C29—H29A	0.9800
C10—H10	0.9500	C29—H29B	0.9800
C11—C12	1.381 (4)	C29—H29C	0.9800
C11—H11	0.9500	C30—H30A	0.9800
C12—C13	1.400 (4)	C30—H30B	0.9800
C12—H12	0.9500	C30—H30C	0.9800
O2—Co1—O1	113.77 (8)	H14B—C14—H14C	109.5
O2—Co1—N2	94.94 (8)	C13—C15—H15A	109.5
O1—Co1—N2	115.58 (8)	C13—C15—H15B	109.5
O2—Co1—N1	116.97 (9)	H15A—C15—H15B	109.5
O1—Co1—N1	94.53 (8)	C13—C15—H15C	109.5
N2—Co1—N1	122.51 (9)	H15A—C15—H15C	109.5
C6—O1—Co1	125.79 (17)	H15B—C15—H15C	109.5
C17—O2—Co1	126.25 (17)	C21—C16—C17	120.0 (2)
C7—N1—C8	117.8 (2)	C21—C16—C22	116.1 (2)
C7—N1—Co1	121.47 (18)	C17—C16—C22	123.9 (2)
C8—N1—Co1	120.72 (17)	O2—C17—C18	119.5 (2)
C22—N2—C23	119.1 (2)	O2—C17—C16	124.3 (2)
C22—N2—Co1	122.70 (18)	C18—C17—C16	116.2 (2)
C23—N2—Co1	118.14 (16)	C19—C18—C17	123.2 (2)
C2—C1—C6	120.7 (2)	C19—C18—Br2	119.1 (2)
C2—C1—C7	116.2 (2)	C17—C18—Br2	117.72 (19)
C6—C1—C7	122.9 (2)	C18—C19—C20	119.0 (2)
C3—C2—C1	120.6 (3)	C18—C19—H19	120.5
C3—C2—H2	119.7	C20—C19—H19	120.5
C1—C2—H2	119.7	C21—C20—C19	120.7 (2)
C2—C3—C4	120.3 (2)	C21—C20—Cl2	120.0 (2)
C2—C3—Cl1	120.3 (2)	C19—C20—Cl2	119.2 (2)
C4—C3—Cl1	119.4 (2)	C20—C21—C16	120.8 (2)



C5—C4—C3	119.0 (2)	C20—C21—H21	119.6
C5—C4—H4	120.5	C16—C21—H21	119.6
C3—C4—H4	120.5	N2—C22—C16	126.2 (2)
C4—C5—C6	123.5 (3)	N2—C22—H22	116.9
C4—C5—Br1	119.0 (2)	C16—C22—H22	116.9
C6—C5—Br1	117.4 (2)	C28—C23—C24	122.0 (3)
O1—C6—C5	119.4 (2)	C28—C23—N2	119.3 (2)
O1—C6—C1	125.1 (2)	C24—C23—N2	118.5 (2)
C5—C6—C1	115.6 (2)	C25—C24—C23	117.4 (3)
N1—C7—C1	127.0 (2)	C25—C24—C29	121.0 (3)
N1—C7—H7	116.5	C23—C24—C29	121.6 (3)
C1—C7—H7	116.5	C26—C25—C24	121.9 (3)
C13—C8—C9	122.2 (2)	C26—C25—H25	119.1
C13—C8—N1	118.7 (2)	C24—C25—H25	119.1
C9—C8—N1	119.0 (2)	C27—C26—C25	119.5 (3)
C10—C9—C8	118.1 (2)	C27—C26—H26	120.2
C10—C9—C14	119.8 (3)	C25—C26—H26	120.2
C8—C9—C14	122.0 (2)	C26—C27—C28	121.5 (3)
C11—C10—C9	120.8 (3)	C26—C27—H27	119.2
C11—C10—H10	119.6	C28—C27—H27	119.2
C9—C10—H10	119.6	C27—C28—C23	117.6 (3)
C12—C11—C10	119.9 (3)	C27—C28—C30	120.7 (3)
C12—C11—H11	120.0	C23—C28—C30	121.7 (3)
C10—C11—H11	120.0	C24—C29—H29A	109.5
C11—C12—C13	121.7 (3)	C24—C29—H29B	109.5
C11—C12—H12	119.2	H29A—C29—H29B	109.5
C13—C12—H12	119.2	C24—C29—H29C	109.5
C8—C13—C12	117.2 (3)	H29A—C29—H29C	109.5
C8—C13—C15	122.5 (2)	H29B—C29—H29C	109.5
C12—C13—C15	120.3 (2)	C28—C30—H30A	109.5
C9—C14—H14A	109.5	C28—C30—H30B	109.5
C9—C14—H14B	109.5	H30A—C30—H30B	109.5
H14A—C14—H14B	109.5	C28—C30—H30C	109.5
C9—C14—H14C	109.5	H30A—C30—H30C	109.5
H14A—C14—H14C	109.5	H30B—C30—H30C	109.5
O2—Co1—O1—C6	106.0 (2)	C14—C9—C10—C11	-177.0 (3)
N2—Co1—O1—C6	-145.6 (2)	C9—C10—C11—C12	-1.0 (5)
N1—Co1—O1—C6	-16.2 (2)	C10—C11—C12—C13	-0.3 (4)
O1—Co1—O2—C17	135.3 (2)	C9—C8—C13—C12	-3.5 (4)
N2—Co1—O2—C17	14.5 (2)	N1—C8—C13—C12	172.1 (2)
N1—Co1—O2—C17	-115.9 (2)	C9—C8—C13—C15	175.2 (3)
O2—Co1—N1—C7	-102.8 (2)	N1—C8—C13—C15	-9.2 (4)
O1—Co1—N1—C7	16.8 (2)	C11—C12—C13—C8	2.5 (4)
N2—Co1—N1—C7	141.1 (2)	C11—C12—C13—C15	-176.1 (3)
O2—Co1—N1—C8	77.5 (2)	Co1—O2—C17—C18	169.79 (18)
O1—Co1—N1—C8	-162.86 (19)	Co1—O2—C17—C16	-11.6 (4)
N2—Co1—N1—C8	-38.5 (2)	C21—C16—C17—O2	-178.5 (2)

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O2—Co1—N2—C22	-10.4 (2)	C22—C16—C17—O2	0.2 (4)
O1—Co1—N2—C22	-129.8 (2)	C21—C16—C17—C18	0.1 (4)
N1—Co1—N2—C22	116.1 (2)	C22—C16—C17—C18	178.8 (2)
O2—Co1—N2—C23	172.64 (18)	O2—C17—C18—C19	178.6 (2)
O1—Co1—N2—C23	53.3 (2)	C16—C17—C18—C19	-0.1 (4)
N1—Co1—N2—C23	-60.8 (2)	O2—C17—C18—Br2	-1.4 (3)
C6—C1—C2—C3	-0.8 (4)	C16—C17—C18—Br2	179.94 (18)
C7—C1—C2—C3	175.6 (2)	C17—C18—C19—C20	-0.2 (4)
C1—C2—C3—C4	-2.7 (4)	Br2—C18—C19—C20	179.80 (19)
C1—C2—C3—Cl1	179.1 (2)	C18—C19—C20—C21	0.4 (4)
C2—C3—C4—C5	2.2 (4)	C18—C19—C20—Cl2	-179.7 (2)
Cl1—C3—C4—C5	-179.6 (2)	C19—C20—C21—C16	-0.4 (4)
C3—C4—C5—C6	1.9 (4)	Cl2—C20—C21—C16	179.75 (19)
C3—C4—C5—Br1	-175.9 (2)	C17—C16—C21—C20	0.1 (4)
Co1—O1—C6—C5	-173.34 (18)	C22—C16—C21—C20	-178.7 (2)
Co1—O1—C6—C1	6.3 (4)	C23—N2—C22—C16	-179.5 (2)
C4—C5—C6—O1	174.4 (3)	Co1—N2—C22—C16	3.6 (4)
Br1—C5—C6—O1	-7.7 (3)	C21—C16—C22—N2	-177.4 (2)
C4—C5—C6—C1	-5.2 (4)	C17—C16—C22—N2	3.8 (4)
Br1—C5—C6—C1	172.68 (19)	C22—N2—C23—C28	-76.9 (3)
C2—C1—C6—O1	-175.1 (3)	Co1—N2—C23—C28	100.1 (2)
C7—C1—C6—O1	8.8 (4)	C22—N2—C23—C24	106.8 (3)
C2—C1—C6—C5	4.5 (4)	Co1—N2—C23—C24	-76.1 (3)
C7—C1—C6—C5	-171.6 (2)	C28—C23—C24—C25	-2.3 (4)
C8—N1—C7—C1	171.2 (2)	N2—C23—C24—C25	173.9 (2)
Co1—N1—C7—C1	-8.4 (4)	C28—C23—C24—C29	177.2 (3)
C2—C1—C7—N1	176.6 (3)	N2—C23—C24—C29	-6.6 (4)
C6—C1—C7—N1	-7.2 (4)	C23—C24—C25—C26	0.1 (4)
C7—N1—C8—C13	110.2 (3)	C29—C24—C25—C26	-179.4 (3)
Co1—N1—C8—C13	-70.2 (3)	C24—C25—C26—C27	1.8 (5)
C7—N1—C8—C9	-74.1 (3)	C25—C26—C27—C28	-1.6 (5)
Co1—N1—C8—C9	105.6 (3)	C26—C27—C28—C23	-0.5 (5)
C13—C8—C9—C10	2.2 (4)	C26—C27—C28—C30	178.3 (3)
N1—C8—C9—C10	-173.4 (2)	C24—C23—C28—C27	2.5 (4)
C13—C8—C9—C14	179.3 (3)	N2—C23—C28—C27	-173.7 (2)
N1—C8—C9—C14	3.7 (4)	C24—C23—C28—C30	-176.3 (3)
C8—C9—C10—C11	0.1 (4)	N2—C23—C28—C30	7.6 (4)

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