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{6,6'-Dimethoxy-2,2'-[*o*-phenylenebis-(nitrilomethyldiylne)]diphenolato}-cobalt(II) dichloromethane disolvate

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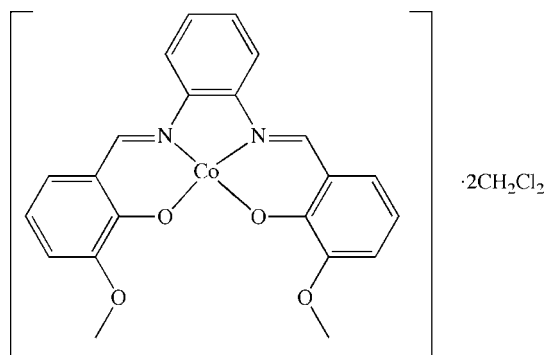
Received 18 December 2008; accepted 8 January 2009

Key indicators: single-crystal X-ray study; $T = 150$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.046; wR factor = 0.089; data-to-parameter ratio = 17.9.

The title compound, $[\text{Co}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)] \cdot 2\text{CH}_2\text{Cl}_2$, was isolated from the reaction of N,N' -(*o*-phenylene)bis(vanillalimine) (H_2L) with $\text{Co}(\text{SCN})_2$. The crystal structure contains a Co^{II} ion surrounded by the L^{2-} ligand in a slightly distorted square-planar fashion. Intermolecular $\text{C}-\text{H} \cdots \text{O}$ hydrogen-bonding contacts between the dichloromethane solvent molecules and the methoxy or carboxylate O atoms are observed in the crystal structure. The planar complex molecules stack through inversion related $\pi-\pi$ interactions between the six-membered rings of the vanillalimine half ligands. The distance between centroids is 3.498 (2) Å and the perpendicular distance is 3.345 Å. A partial stacking is observed with a centroid-centroid distance of 3.830 (2) Å, a perpendicular distance of 3.350 Å and a slippage of 1.856 Å.

Related literature

For general background, see: Cotton *et al.* (1999); Liu *et al.* (2007); Sharghi & Al Nasser (2003). For related structures, see: Pahor *et al.* (1976). For related properties, see: Bella *et al.* (1995).



Experimental

Crystal data

$[\text{Co}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)] \cdot 2\text{CH}_2\text{Cl}_2$

$M_r = 603.19$

Monoclinic, $P2_1/a$

$a = 13.309$ (6) Å

$b = 14.088$ (6) Å

$c = 14.101$ (6) Å

$\beta = 109.676$ (6)°

$V = 2489.4$ (19) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.15$ mm⁻¹

$T = 150$ (1) K

$0.50 \times 0.30 \times 0.10$ mm

Data collection

Rigaku Mercury diffractometer

Absorption correction: multi-scan

(*REQAB*; Jacobson, 1998)

$T_{\text{min}} = 0.764$, $T_{\text{max}} = 0.891$

28457 measured reflections

5677 independent reflections

5100 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.040$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$

$wR(F^2) = 0.089$

$S = 1.15$

5677 reflections

317 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.53$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.66$ e Å⁻³

Table 1

Selected bond lengths (Å).

Co1—O1	1.8593 (15)	Co1—N1	1.8807 (17)
Co1—O2	1.8611 (14)	Co1—N2	1.8755 (18)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
C23—H23A \cdots O3	0.99	2.54	3.472 (4)	158
C23—H23B \cdots O4	0.99	2.33	3.252 (4)	154
C23—H23B \cdots O2	0.99	2.41	3.202 (3)	137
C24—H24A \cdots O3	0.99	2.35	3.173 (4)	140
C24—H24B \cdots O4	0.99	2.38	3.250 (4)	147

Data collection: *CrystalClear* (Rigaku/MSK, 2007); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSK, 2007); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2147).

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supporting information

Acta Cryst. (2009). E65, m188–m189 [doi:10.1107/S160053680900083X]

{6,6'-Dimethoxy-2,2'-[o-phenylenebis(nitrilomethylidyne)]diphenolato}cobalt(II) dichloromethane disolvate

Atsuhiko Nabei, Takayoshi Kuroda-Sowa, Takashi Okubo, Masahiko Maekawa and Megumu Munakata

S1. Comment

Cobalt–Schiff base complexes are thoroughly investigated in their catalytic oxidation, chiral synthesis in solution, and so on (Cotton *et al.*, 1999; Liu *et al.*, 2007; Sharghi *et al.*, 2003). However, a relatively few works are devoted to their solid state properties such as magnetic or conductive properties (Bella *et al.*, 1995). Our interest on the cobalt-salophen system is based on their planar structure (Pahor *et al.*, 1976) together with its redox-active characteristics, which implies their potential application for conducting and/or magnetic devices. In this work the structure of the title molecule, $[\text{Co}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)]_2(\text{CH}_2\text{Cl}_2)$ is reported (Fig. 1) The coordination sphere around Co^{II} ions is square planar and made up of equatorial planar N_2O_2 coordination from L^2 . The Co—O and Co—N bond distances are given in Table 1. The Co—N distances are comparable to those of low spin (LS) Co^{II} species, representing a characteristic feature of the LS state. Intermolecular C—H \cdots O hydrogen bonding contacts are observed in the title structure (Table 2) between methoxy oxygen atoms and the dichloromethane donors. The planar molecules stack each other through inversion related $\pi\cdots\pi$ interactions, with the centroids $\text{Cg}3\cdots\text{Cg}6^i$ distance of 3.498 (2) Å, the perpendicular distance of the centroid $\text{Cg}3$ and the plane of $\text{Cg}6$ is 3.345 Å; a partial stacking is also observed between inversion related $\text{Cg}3$ rings: $\text{Cg}3\cdots\text{Cg}3^i = 3.830$ (2) Å, the perpendicular distance is 3.350 Å, the slippage between rings is 1.856 Å, symmetry code $i = -x, -y, 1 - z$. definitions: $\text{Cg}3$ is the centroid of the ring Co, O2, C21, C16, C15, N2 $\text{Cg}6$ is the centroid of the ring C16 - C21

S2. Experimental

To a dichloromethane solution (10 ml) containing H_2L (0.1 mmol, 42.7 mg) placed at the bottom of a glass tube, a methanol solution (10 ml) containing $\text{Co}(\text{SCN})_2$ (0.1 mmol, 17.6 mg) was added quietly. After standing for two weeks at room temperature, brown brick crystals of (I) suitable for X-ray analysis were obtained.

S3. Refinement

All H atoms were positioned geometrically and treated as riding [C—H = 0.95 Å, 0.98 Å and 0.99 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

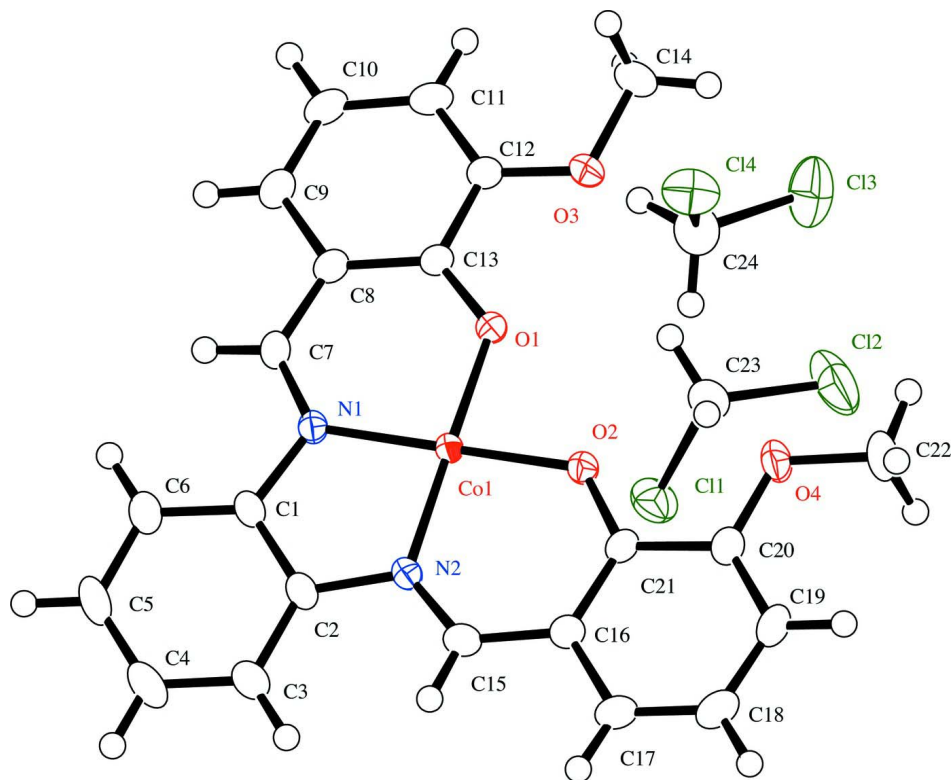


Figure 1

The molecular structure of (I), with the atom-numbering scheme, showing 50% probability displacement ellipsoids.

{6,6'-Dimethoxy-2,2'-[o-phenylenebis(nitrilomethylidene)]diphenolato}cobalt(II) dichloromethane disolvate

Crystal data

$[\text{Co}(\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_4)] \cdot 2\text{CH}_2\text{Cl}_2$

$M_r = 603.19$

Monoclinic, $P2_1/a$

Hall symbol: $-P\ 2yab$

$a = 13.309\ (6)\ \text{\AA}$

$b = 14.088\ (6)\ \text{\AA}$

$c = 14.101\ (6)\ \text{\AA}$

$\beta = 109.676\ (6)^\circ$

$V = 2489.4\ (19)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1228.00$

$D_x = 1.609\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71070\ \text{\AA}$

Cell parameters from 6959 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 1.15\ \text{mm}^{-1}$

$T = 150\ \text{K}$

Block, brown

$0.50 \times 0.30 \times 0.10\ \text{mm}$

Data collection

Rigaku Mercury
diffractometer

Detector resolution: $7.31\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*REQAB*; Jacobson, 1998)

$T_{\min} = 0.764$, $T_{\max} = 0.891$

28457 measured reflections

5677 independent reflections

5100 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.040$

$\theta_{\text{max}} = 27.5^\circ$

$h = -17 \rightarrow 17$

$k = -18 \rightarrow 17$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.089$
 $S = 1.15$
 5677 reflections
 317 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 1.9552P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.66 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. The planar Co^{II} complex has non-crystallographic mm2 symmetry.

Refinement. Refinement was performed using all reflections. The weighted R -factor (wR) and goodness of fit (S) are based on F^2 . R -factor (gt) are based on F . The threshold expression of $F^2 > 2.0 \sigma(F^2)$ is used only for calculating R -factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.13131 (2)	0.19517 (2)	0.52772 (2)	0.01696 (7)
Cl1	0.44427 (5)	0.14026 (5)	0.68960 (5)	0.03951 (16)
Cl2	0.47220 (7)	0.09420 (8)	0.89664 (6)	0.0672 (2)
Cl3	0.21820 (7)	0.13146 (7)	0.96127 (7)	0.0621 (2)
Cl4	-0.00594 (6)	0.12289 (5)	0.83886 (6)	0.04414 (17)
O1	0.17603 (12)	0.26802 (11)	0.64445 (11)	0.0208 (3)
O2	0.16176 (12)	0.08953 (10)	0.61189 (11)	0.0208 (3)
O3	0.24984 (13)	0.33830 (12)	0.82700 (11)	0.0269 (3)
O4	0.21621 (14)	-0.03363 (12)	0.75913 (12)	0.0310 (3)
N1	0.09468 (14)	0.30090 (13)	0.44144 (13)	0.0186 (3)
N2	0.09571 (14)	0.12300 (13)	0.40921 (13)	0.0186 (3)
C1	0.05949 (17)	0.27635 (16)	0.33749 (16)	0.0202 (4)
C2	0.06502 (17)	0.17945 (16)	0.32009 (16)	0.0207 (4)
C3	0.04319 (19)	0.14651 (18)	0.22208 (17)	0.0277 (5)
C4	0.0107 (2)	0.2098 (2)	0.14228 (18)	0.0329 (5)
C5	-0.00149 (19)	0.3053 (2)	0.15966 (18)	0.0315 (5)
C6	0.02351 (19)	0.33956 (18)	0.25698 (18)	0.0273 (5)
C7	0.10471 (17)	0.39009 (16)	0.46840 (17)	0.0218 (4)
C8	0.14351 (17)	0.42339 (16)	0.56916 (17)	0.0210 (4)
C9	0.14867 (19)	0.52326 (16)	0.58418 (19)	0.0271 (5)
C10	0.1866 (2)	0.56020 (17)	0.6785 (2)	0.0301 (5)
C11	0.22151 (19)	0.49922 (17)	0.76248 (19)	0.0279 (5)
C12	0.21817 (17)	0.40256 (16)	0.74993 (17)	0.0215 (4)
C13	0.17848 (17)	0.36031 (15)	0.65197 (16)	0.0187 (4)
C14	0.2753 (2)	0.3763 (2)	0.92607 (18)	0.0356 (6)
C15	0.09237 (17)	0.03043 (17)	0.40283 (17)	0.0226 (4)
C16	0.12100 (17)	-0.03338 (16)	0.48546 (17)	0.0206 (4)
C17	0.11515 (19)	-0.13206 (16)	0.46470 (19)	0.0261 (5)
C18	0.14356 (19)	-0.19674 (17)	0.5414 (2)	0.0293 (5)
C19	0.17852 (19)	-0.16544 (17)	0.64144 (19)	0.0270 (5)
C20	0.18411 (18)	-0.07012 (16)	0.66371 (17)	0.0227 (4)
C21	0.15525 (17)	0.00007 (15)	0.58599 (16)	0.0193 (4)

C22	0.2476 (2)	-0.09938 (19)	0.84100 (19)	0.0353 (6)
C23	0.38345 (19)	0.14048 (19)	0.78310 (18)	0.0298 (5)
C24	0.1234 (2)	0.1508 (2)	0.8408 (2)	0.0408 (6)
H3	0.0505	0.0810	0.2100	0.033*
H4	-0.0033	0.1877	0.0754	0.039*
H5	-0.0272	0.3476	0.1043	0.038*
H6	0.0162	0.4052	0.2687	0.033*
H7	0.0844	0.4363	0.4164	0.026*
H9	0.1254	0.5646	0.5277	0.033*
H10	0.1896	0.6271	0.6879	0.036*
H11	0.2476	0.5253	0.8284	0.034*
H14A	0.2969	0.3247	0.9754	0.043*
H14B	0.2125	0.4084	0.9323	0.043*
H14C	0.3339	0.4219	0.9385	0.043*
H15	0.0687	0.0036	0.3372	0.027*
H17	0.0912	-0.1534	0.3968	0.031*
H18	0.1396	-0.2628	0.5268	0.035*
H19	0.1986	-0.2106	0.6946	0.032*
H22A	0.2687	-0.0645	0.9049	0.042*
H22B	0.3081	-0.1372	0.8375	0.042*
H22C	0.1877	-0.1415	0.8368	0.042*
H23A	0.3633	0.2061	0.7942	0.036*
H23B	0.3177	0.1015	0.7605	0.036*
H24A	0.1258	0.2182	0.8216	0.049*
H24B	0.1414	0.1111	0.7908	0.049*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02030 (15)	0.01570 (15)	0.01475 (14)	0.00061 (12)	0.00574 (11)	0.00093 (11)
Cl1	0.0392 (3)	0.0514 (4)	0.0337 (3)	0.0015 (3)	0.0199 (2)	0.0022 (3)
Cl2	0.0516 (4)	0.1169 (8)	0.0295 (3)	0.0179 (5)	0.0088 (3)	0.0173 (4)
Cl3	0.0503 (4)	0.0594 (5)	0.0615 (5)	0.0012 (4)	-0.0009 (3)	0.0198 (4)
Cl4	0.0392 (3)	0.0473 (4)	0.0512 (4)	-0.0109 (3)	0.0223 (3)	-0.0102 (3)
O1	0.0281 (8)	0.0165 (7)	0.0177 (7)	0.0011 (6)	0.0075 (6)	0.0001 (6)
O2	0.0258 (8)	0.0177 (7)	0.0178 (7)	-0.0001 (6)	0.0062 (6)	0.0002 (6)
O3	0.0367 (9)	0.0249 (8)	0.0172 (7)	0.0024 (7)	0.0066 (6)	-0.0028 (6)
O4	0.0449 (10)	0.0263 (9)	0.0203 (8)	0.0014 (7)	0.0089 (7)	0.0072 (6)
N1	0.0183 (8)	0.0200 (9)	0.0176 (8)	0.0018 (7)	0.0064 (7)	0.0030 (7)
N2	0.0185 (8)	0.0214 (9)	0.0160 (8)	0.0001 (7)	0.0059 (6)	0.0011 (7)
C1	0.0170 (10)	0.0269 (11)	0.0164 (10)	-0.0008 (8)	0.0050 (8)	0.0029 (8)
C2	0.0172 (10)	0.0277 (12)	0.0168 (10)	-0.0018 (8)	0.0051 (8)	0.0024 (8)
C3	0.0299 (12)	0.0314 (13)	0.0199 (11)	-0.0034 (10)	0.0061 (9)	-0.0020 (9)
C4	0.0300 (13)	0.0490 (16)	0.0174 (11)	-0.0070 (11)	0.0049 (9)	0.0015 (10)
C5	0.0289 (12)	0.0431 (15)	0.0197 (11)	-0.0016 (11)	0.0046 (9)	0.0106 (10)
C6	0.0264 (12)	0.0315 (12)	0.0236 (11)	0.0013 (10)	0.0077 (9)	0.0068 (10)
C7	0.0212 (10)	0.0225 (11)	0.0223 (11)	0.0021 (9)	0.0082 (8)	0.0062 (8)
C8	0.0193 (10)	0.0189 (11)	0.0269 (11)	0.0006 (8)	0.0104 (9)	0.0006 (9)

C9	0.0289 (12)	0.0197 (11)	0.0326 (13)	0.0016 (9)	0.0103 (10)	0.0029 (9)
C10	0.0347 (13)	0.0162 (11)	0.0401 (14)	-0.0005 (10)	0.0135 (11)	-0.0049 (10)
C11	0.0282 (12)	0.0244 (12)	0.0312 (12)	-0.0008 (10)	0.0099 (10)	-0.0094 (10)
C12	0.0205 (10)	0.0224 (11)	0.0230 (10)	0.0011 (9)	0.0090 (8)	-0.0016 (9)
C13	0.0168 (10)	0.0188 (11)	0.0220 (10)	0.0008 (8)	0.0084 (8)	-0.0006 (8)
C14	0.0459 (15)	0.0377 (14)	0.0208 (11)	0.0024 (12)	0.0078 (11)	-0.0074 (10)
C15	0.0211 (11)	0.0250 (11)	0.0224 (11)	-0.0022 (9)	0.0083 (8)	-0.0042 (9)
C16	0.0183 (10)	0.0208 (11)	0.0236 (10)	-0.0014 (8)	0.0084 (8)	-0.0010 (9)
C17	0.0270 (12)	0.0207 (11)	0.0321 (12)	-0.0029 (9)	0.0119 (10)	-0.0066 (9)
C18	0.0299 (13)	0.0179 (11)	0.0429 (14)	-0.0014 (10)	0.0162 (11)	-0.0013 (10)
C19	0.0283 (12)	0.0192 (11)	0.0361 (13)	0.0025 (9)	0.0141 (10)	0.0089 (9)
C20	0.0205 (11)	0.0223 (11)	0.0267 (11)	0.0007 (9)	0.0099 (9)	0.0044 (9)
C21	0.0167 (10)	0.0169 (10)	0.0252 (11)	0.0004 (8)	0.0084 (8)	0.0011 (8)
C22	0.0393 (14)	0.0388 (15)	0.0277 (12)	0.0043 (12)	0.0109 (11)	0.0156 (11)
C23	0.0251 (12)	0.0379 (14)	0.0265 (12)	-0.0005 (10)	0.0090 (9)	-0.0011 (10)
C24	0.0342 (14)	0.0486 (17)	0.0425 (15)	0.0010 (13)	0.0169 (12)	0.0072 (13)

Geometric parameters (Å, °)

Co1—O1	1.8593 (15)	C12—C13	1.432 (3)
Co1—O2	1.8611 (14)	C15—C16	1.418 (3)
Co1—N1	1.8807 (17)	C16—C17	1.417 (3)
Co1—N2	1.8755 (18)	C16—C21	1.416 (3)
C11—C23	1.764 (3)	C17—C18	1.366 (3)
C12—C23	1.764 (2)	C18—C19	1.400 (3)
C13—C24	1.764 (2)	C19—C20	1.375 (3)
C14—C24	1.757 (3)	C20—C21	1.429 (3)
O1—C13	1.304 (2)	C3—H3	0.950
O2—C21	1.307 (2)	C4—H4	0.950
O3—C12	1.367 (2)	C5—H5	0.950
O3—C14	1.426 (2)	C6—H6	0.950
O4—C20	1.367 (2)	C7—H7	0.950
O4—C22	1.428 (3)	C9—H9	0.950
N1—C1	1.423 (2)	C10—H10	0.950
N1—C7	1.306 (2)	C11—H11	0.950
N2—C2	1.426 (2)	C14—H14A	0.980
N2—C15	1.307 (3)	C14—H14B	0.980
C1—C2	1.393 (3)	C14—H14C	0.980
C1—C6	1.395 (3)	C15—H15	0.950
C2—C3	1.393 (3)	C17—H17	0.950
C3—C4	1.386 (3)	C18—H18	0.950
C4—C5	1.386 (3)	C19—H19	0.950
C5—C6	1.386 (3)	C22—H22A	0.980
C7—C8	1.418 (3)	C22—H22B	0.980
C8—C9	1.421 (3)	C22—H22C	0.980
C8—C13	1.416 (3)	C23—H23A	0.990
C9—C10	1.358 (3)	C23—H23B	0.990
C10—C11	1.409 (3)	C24—H24A	0.990

C11—C12	1.372 (3)	C24—H24B	0.990
O1—Co1—O2	86.60 (6)	O2—C21—C20	118.52 (19)
O1—Co1—N1	94.10 (7)	C16—C21—C20	116.76 (19)
O1—Co1—N2	175.97 (8)	C11—C23—C12	110.01 (14)
O2—Co1—N1	177.70 (7)	C13—C24—C14	111.07 (18)
O2—Co1—N2	94.02 (7)	C2—C3—H3	120.2
N1—Co1—N2	85.43 (7)	C4—C3—H3	120.2
Co1—O1—C13	127.89 (13)	C3—C4—H4	119.9
Co1—O2—C21	127.82 (13)	C5—C4—H4	119.9
C12—O3—C14	115.96 (18)	C4—C5—H5	119.7
C20—O4—C22	117.44 (18)	C6—C5—H5	119.7
Co1—N1—C1	113.43 (14)	C1—C6—H6	120.5
Co1—N1—C7	126.48 (14)	C5—C6—H6	120.5
C1—N1—C7	119.96 (18)	N1—C7—H7	117.4
Co1—N2—C2	113.23 (14)	C8—C7—H7	117.4
Co1—N2—C15	126.50 (15)	C8—C9—H9	119.7
C2—N2—C15	120.19 (18)	C10—C9—H9	119.7
N1—C1—C2	113.64 (18)	C9—C10—H10	120.1
N1—C1—C6	125.9 (2)	C11—C10—H10	120.1
C2—C1—C6	120.4 (2)	C10—C11—H11	119.7
N2—C2—C1	114.06 (19)	C12—C11—H11	119.7
N2—C2—C3	126.2 (2)	O3—C14—H14A	109.5
C1—C2—C3	119.7 (2)	O3—C14—H14B	109.5
C2—C3—C4	119.7 (2)	O3—C14—H14C	109.5
C3—C4—C5	120.3 (2)	H14A—C14—H14B	109.5
C4—C5—C6	120.7 (2)	H14A—C14—H14C	109.5
C1—C6—C5	119.1 (2)	H14B—C14—H14C	109.5
N1—C7—C8	125.2 (2)	N2—C15—H15	117.2
C7—C8—C9	117.4 (2)	C16—C15—H15	117.2
C7—C8—C13	121.8 (2)	C16—C17—H17	119.7
C9—C8—C13	120.8 (2)	C18—C17—H17	119.7
C8—C9—C10	120.6 (2)	C17—C18—H18	120.1
C9—C10—C11	119.9 (2)	C19—C18—H18	120.1
C10—C11—C12	120.6 (2)	C18—C19—H19	119.6
O3—C12—C11	124.5 (2)	C20—C19—H19	119.6
O3—C12—C13	113.98 (18)	O4—C22—H22A	109.5
C11—C12—C13	121.5 (2)	O4—C22—H22B	109.5
O1—C13—C8	124.51 (19)	O4—C22—H22C	109.5
O1—C13—C12	118.94 (18)	H22A—C22—H22B	109.5
C8—C13—C12	116.54 (19)	H22A—C22—H22C	109.5
N2—C15—C16	125.6 (2)	H22B—C22—H22C	109.5
C15—C16—C17	118.1 (2)	C11—C23—H23A	109.7
C15—C16—C21	121.2 (2)	C11—C23—H23B	109.7
C17—C16—C21	120.7 (2)	C12—C23—H23A	109.7
C16—C17—C18	120.6 (2)	C12—C23—H23B	109.7
C17—C18—C19	119.8 (2)	H23A—C23—H23B	108.2
C18—C19—C20	120.8 (2)	C13—C24—H24A	109.4

O4—C20—C19	124.5 (2)	C13—C24—H24B	109.4
O4—C20—C21	114.12 (19)	C14—C24—H24A	109.4
C19—C20—C21	121.4 (2)	C14—C24—H24B	109.4
O2—C21—C16	124.72 (19)	H24A—C24—H24B	108.0
O1—Co1—O2—C21	-176.86 (19)	N2—C2—C3—C4	177.9 (2)
O2—Co1—O1—C13	-178.94 (19)	C1—C2—C3—C4	-3.4 (3)
O1—Co1—N1—C1	176.77 (15)	C2—C3—C4—C5	-0.9 (3)
O1—Co1—N1—C7	1.0 (2)	C3—C4—C5—C6	3.2 (4)
N1—Co1—O1—C13	-1.1 (2)	C4—C5—C6—C1	-1.1 (3)
O2—Co1—N2—C2	179.84 (15)	N1—C7—C8—C9	-179.9 (2)
O2—Co1—N2—C15	3.2 (2)	N1—C7—C8—C13	1.7 (3)
N2—Co1—O2—C21	-0.85 (19)	C7—C8—C9—C10	-178.9 (2)
N1—Co1—N2—C2	2.08 (15)	C7—C8—C13—O1	-1.9 (3)
N1—Co1—N2—C15	-174.6 (2)	C7—C8—C13—C12	178.6 (2)
N2—Co1—N1—C1	0.78 (16)	C9—C8—C13—O1	179.8 (2)
N2—Co1—N1—C7	-175.0 (2)	C9—C8—C13—C12	0.3 (3)
Co1—O1—C13—C8	1.8 (3)	C13—C8—C9—C10	-0.5 (3)
Co1—O1—C13—C12	-178.74 (16)	C8—C9—C10—C11	0.2 (3)
Co1—O2—C21—C16	-1.1 (3)	C9—C10—C11—C12	0.4 (4)
Co1—O2—C21—C20	179.16 (16)	C10—C11—C12—O3	-179.6 (2)
C14—O3—C12—C11	7.9 (3)	C10—C11—C12—C13	-0.6 (3)
C14—O3—C12—C13	-171.2 (2)	O3—C12—C13—O1	-0.1 (2)
C22—O4—C20—C19	1.1 (3)	O3—C12—C13—C8	179.4 (2)
C22—O4—C20—C21	-179.3 (2)	C11—C12—C13—O1	-179.3 (2)
Co1—N1—C1—C2	-3.6 (2)	C11—C12—C13—C8	0.3 (3)
Co1—N1—C1—C6	177.4 (2)	N2—C15—C16—C17	-178.4 (2)
Co1—N1—C7—C8	-1.4 (3)	N2—C15—C16—C21	1.2 (3)
C1—N1—C7—C8	-177.0 (2)	C15—C16—C17—C18	178.8 (2)
C7—N1—C1—C2	172.6 (2)	C15—C16—C21—O2	1.3 (3)
C7—N1—C1—C6	-6.5 (3)	C15—C16—C21—C20	-178.9 (2)
Co1—N2—C2—C1	-4.6 (2)	C17—C16—C21—O2	-179.1 (2)
Co1—N2—C2—C3	174.2 (2)	C17—C16—C21—C20	0.7 (3)
Co1—N2—C15—C16	-3.7 (3)	C21—C16—C17—C18	-0.7 (3)
C2—N2—C15—C16	179.8 (2)	C16—C17—C18—C19	0.2 (3)
C15—N2—C2—C1	172.3 (2)	C17—C18—C19—C20	0.4 (4)
C15—N2—C2—C3	-8.9 (3)	C18—C19—C20—O4	179.3 (2)
N1—C1—C2—N2	5.3 (2)	C18—C19—C20—C21	-0.4 (3)
N1—C1—C2—C3	-173.6 (2)	O4—C20—C21—O2	-0.0 (2)
N1—C1—C6—C5	175.8 (2)	O4—C20—C21—C16	-179.8 (2)
C2—C1—C6—C5	-3.2 (3)	C19—C20—C21—O2	179.7 (2)
C6—C1—C2—N2	-175.6 (2)	C19—C20—C21—C16	-0.1 (2)
C6—C1—C2—C3	5.5 (3)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C23—H23 <i>A</i> ...O3	0.99	2.54	3.472 (4)	158

supporting information

C23—H23B···O4	0.99	2.33	3.252 (4)	154
C23—H23B···O2	0.99	2.41	3.202 (3)	137
C24—H24A···O3	0.99	2.35	3.173 (4)	140
C24—H24B···O4	0.99	2.38	3.250 (4)	147
