

$[\mu$ -1,2-Bis(2-hydroxybenzoyl)-hydrazine(4-)]bis[tripyridinecobalt(II)] bis[trichloridopyridinecobalt(III)]

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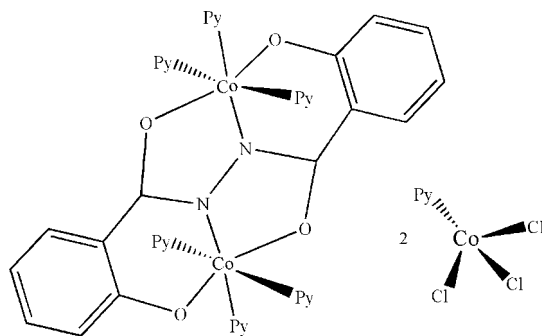
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; R factor = 0.064; wR factor = 0.161; data-to-parameter ratio = 14.6.

The title complex is composed of two different structural units, $[\text{Co}_2(\text{C}_{14}\text{H}_8\text{N}_2\text{O}_4)(\text{C}_5\text{H}_5\text{N})_6] \cdot [\text{CoCl}_3(\text{C}_5\text{H}_5\text{N})]_2$ or $A \cdot 2B$. The A unit is centrosymmetric. Each Co^{II} atom in A exhibits a distorted octahedral $\text{Co}(\text{ONO})(\text{N})(\text{N})(\text{N})$ coordination environment, and the $\text{Co}^{\text{II}} \cdots \text{Co}^{\text{II}}$ distance is 4.409 (3) Å, whereas the cobalt(III) ion in B displays a distorted tetrahedral geometry. Group A is assembled into a two-dimensional network *via* intermolecular $\text{C}-\text{H} \cdots \pi$ interactions along the [101] direction.

Related literature

Three manganese metallacrowns with unsymmetrical aryl-hydrazine ligands were synthesized and reported by Dou *et al.* (2006) and John *et al.* (2006). For the crystal structure of an iron compound with N,N' -bis-picolinoylhydrazine, see: Bernhardt *et al.* (2005). For a nickel complex of N,N' -bis-salicyloylhydrazine, see: Chen *et al.* (2007).



Experimental

Crystal data

$[\text{Co}_2(\text{C}_{14}\text{H}_8\text{N}_2\text{O}_4)(\text{C}_5\text{H}_5\text{N})_6] \cdot [\text{CoCl}_3(\text{C}_5\text{H}_5\text{N})]_2$
 $M_r = 1349.44$
 Monoclinic, $P2_1/n$
 $a = 16.5112$ (18) Å
 $b = 10.7135$ (15) Å
 $c = 17.975$ (2) Å
 $\beta = 66.078$ (2)°
 $V = 2906.6$ (6) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.45$ mm⁻¹
 $T = 298$ (2) K
 $0.43 \times 0.24 \times 0.20$ mm

Data collection

Bruker SMART 1000 CCD area detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.574$, $T_{\max} = 0.760$
 14302 measured reflections
 5138 independent reflections
 2342 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.097$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.161$
 $S = 1.00$
 5138 reflections
 352 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.84$ e Å⁻³
 $\Delta\rho_{\min} = -0.35$ e Å⁻³

Table 1
Selected bond lengths (Å).

Co1—N1 ⁱ	1.848 (5)	Co1—N4	1.964 (5)
Co1—O2 ^j	1.853 (4)	Co2—N5	2.046 (7)
Co1—O1	1.914 (4)	Co2—Cl3	2.204 (2)
Co1—N3	1.945 (5)	Co2—Cl2	2.221 (2)
Co1—N2	1.960 (5)	Co2—Cl1	2.230 (2)

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

Table 2

$\text{C}-\text{H} \cdots \pi$ weak interaction parameters (Å, °).

C_g is the centroid of the C2–C7 ring.

$\text{C}-\text{H} \cdots C_g$	$\text{C}-\text{H}$	$\text{H} \cdots C_g$	$\text{C} \cdots C_g$	$\text{C}-\text{H} \cdots C_g$
C20—H20 ⁱⁱ $\cdots C_g^{\text{ii}}$	0.93	2.64	3.327 (4)	132

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2146).

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**[μ -1,2-Bis(2-hydroxybenzoyl)hydrazine(4-)]bis[tripyridinecobalt(II)]
bis[trichloridopyridinecobalt(III)]**

Y.-T. Chen, J.-M. Dou, D.-C. Li, D.-Q. Wang and Y.-H. Zhu

Comment

A large number of aroylhydrazine complexes have been prepared and studied due to their diverse molecular architectures and quite interesting chemical properties (Dou *et al.*, 2006; John *et al.*, 2006). However, only a few of the compounds with symmetrical diaroylhydrazine ligands have so far been reported (Bernhardt *et al.*, 2005; Chen *et al.*, 2007). Herein, we have synthesized and solve the crystal structure of a new cobalt complex with N, N'-bis-salicyloylhydrazine (I).

The title complex consists of two structural units: [Co₂(C₁₄H₈N₂O₄)(C₅H₅N)₆](A) and [CoCl₃(C₅H₅N)](B). The unit (A) exhibits crystallographic inversion symmetry and is composed of a tetranionic hexadentate ligand bridging two cobalt(II) ions and six pyridine molecules. The distance Co^{II}...Co^{II} is 4.409 Å. As shown in Table 1, each cobalt(II) ion in the unit (A) is in a slightly distorted octahedral coordination constructed by three pyridine N, along with a phenolate O, a carbonyl O and a hydrazine N of the ligand which form the fused five-membered and six-membered rings with the cobalt(II) ion. These two unique chelate rings are near to coplanar with a dihedral angle of 3(4)°. The unit (B) contains a cobalt(III) ion, three chloride ions and the N-coordinated pyridine molecule (Fig. 1, Table 1). The units (A) are linked into two-dimensional network by intermolecular C—H... π interactions between two aromatic rings [C20—H20...Cgⁱⁱ with H...Cgⁱⁱ of 2.636 Å and C—H...Cg angle of 131.59°, Cg is a centroid of C2→C7 with symmetry code: (ii) 0.5 - x, 1/2 + y, -0.5 - z] along the direction [101] (Fig. 2).

Experimental

The solution of CoCl₂·4H₂O (0.04 g, 0.2 mmol) in methanol (10 ml) was added to the mixture of N, N'-disalicyloylhydrazine (0.027 g, 0.1 mmol) and sodium hydroxide (0.016 g, 0.4 mmol) in pyridine (10 ml). A black-green solution was obtained after refluxing for 1 h. After filtrated, dimethyl ether was slowly diffused into the filtrate. Black-green block crystals suitable for X-ray diffraction were obtained after five days. Yield: 0.0387 g, 57.38%. m. p. > 573 K. Anal. for C₅₄H₄₈Cl₆Co₄N₁₀O₄: Calc. C, 48.02; H, 3.56; N, 10.374; Found: C, 48.21; H, 3.49; N, 10.58%.

Refinement

The H atoms on the ligands were allowed to ride on their parent atoms with C(sp² hybrid)-H distances of 0.93 Å (*U*_{iso}(H)=1.2*U*_{eq}(C)) and C(Pyridine)-H distance of 0.93 Å (*U*_{iso}(H)=1.2*U*_{eq}(C)).

Figures

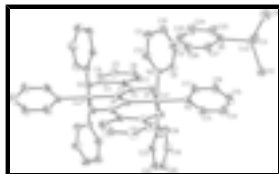


Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. symmetry code (i): $-x, 1 - y, -z$.

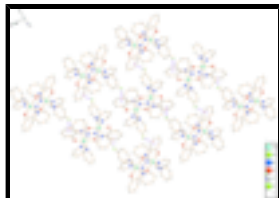


Fig. 2. Two-dimensional network of the complex unit (A) generated by C—H... π interactions between aromatic rings [symm (ii): $0.5 - x, 1/2 + y, -0.5 - z$].

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Crystal data

$[\text{Co}_2(\text{C}_{14}\text{H}_8\text{N}_2\text{O}_4)(\text{C}_5\text{H}_5\text{N})_6][\text{CoCl}_3(\text{C}_5\text{H}_5\text{N})]_2$	$F_{000} = 1368$
$M_r = 1349.44$	$D_x = 1.542 \text{ Mg m}^{-3}$
Monoclinic, $P2(1)/n$	Mo $K\alpha$ radiation
Hall symbol: $-P 2_1n$	$\lambda = 0.71073 \text{ \AA}$
$a = 16.5112 (18) \text{ \AA}$	Cell parameters from 2199 reflections
$b = 10.7135 (15) \text{ \AA}$	$\theta = 2.3\text{--}21.3^\circ$
$c = 17.975 (2) \text{ \AA}$	$\mu = 1.45 \text{ mm}^{-1}$
$\beta = 66.078 (2)^\circ$	$T = 298 (2) \text{ K}$
$V = 2906.6 (6) \text{ \AA}^3$	Block, black-green
$Z = 2$	$0.43 \times 0.24 \times 0.20 \text{ mm}$

Data collection

Bruker SMART 1000 CCD area detector diffractometer	5138 independent reflections
Radiation source: fine-focus sealed tube	2342 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.097$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.4^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -19 \rightarrow 19$
$T_{\text{min}} = 0.574, T_{\text{max}} = 0.760$	$k = -7 \rightarrow 12$
14302 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
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Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.064$$

$$wR(F^2) = 0.161$$

$$S = 1.00$$

5138 reflections

352 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.060P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.84 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.35 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.07028 (5)	0.35002 (9)	0.03356 (5)	0.0496 (3)
Co2	0.47639 (6)	0.40056 (11)	0.18083 (6)	0.0736 (4)
Cl1	0.42810 (14)	0.3642 (3)	0.31408 (13)	0.1100 (9)
Cl2	0.48920 (14)	0.2301 (2)	0.10663 (14)	0.0947 (7)
Cl3	0.59998 (13)	0.5098 (2)	0.12956 (17)	0.1122 (9)
N1	0.0141 (3)	0.5589 (4)	-0.0139 (3)	0.0479 (14)
N2	0.0166 (3)	0.3879 (5)	0.1503 (3)	0.0469 (13)
N3	0.1655 (3)	0.2636 (6)	0.0496 (3)	0.0527 (14)
N4	0.1304 (3)	0.3071 (5)	-0.0823 (3)	0.0491 (14)
N5	0.3818 (5)	0.5125 (8)	0.1692 (5)	0.091 (2)
O1	0.1324 (2)	0.5058 (4)	0.0098 (2)	0.0517 (11)
O2	-0.0026 (3)	0.7940 (4)	-0.0541 (2)	0.0566 (12)
C1	0.0910 (4)	0.5862 (7)	-0.0139 (3)	0.0486 (17)
C2	0.1269 (4)	0.7078 (7)	-0.0411 (3)	0.0497 (17)
C3	0.0803 (4)	0.7996 (7)	-0.0610 (4)	0.0511 (17)
C4	0.1220 (5)	0.9097 (8)	-0.0894 (4)	0.073 (2)
H4	0.0914	0.9722	-0.1032	0.088*
C5	0.2074 (6)	0.9329 (9)	-0.0988 (5)	0.087 (3)
H5	0.2338	1.0093	-0.1192	0.105*
C6	0.2537 (5)	0.8424 (9)	-0.0779 (5)	0.078 (2)
H6	0.3114	0.8573	-0.0836	0.093*
C7	0.2144 (4)	0.7325 (7)	-0.0490 (4)	0.0590 (19)

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H7	0.2450	0.6716	-0.0340	0.071*
C8	0.0009 (5)	0.2965 (7)	0.2040 (4)	0.066 (2)
H8	0.0118	0.2146	0.1855	0.079*
C9	-0.0313 (5)	0.3193 (8)	0.2868 (5)	0.080 (2)
H9	-0.0434	0.2544	0.3242	0.096*
C10	-0.0442 (6)	0.4391 (9)	0.3111 (5)	0.087 (3)
H10	-0.0629	0.4579	0.3661	0.105*
C11	-0.0307 (5)	0.5311 (8)	0.2577 (5)	0.081 (2)
H11	-0.0432	0.6133	0.2752	0.097*
C12	0.0020 (5)	0.5029 (8)	0.1765 (4)	0.065 (2)
H12	0.0141	0.5675	0.1390	0.078*
C13	0.1702 (5)	0.1428 (8)	0.0509 (4)	0.068 (2)
H13	0.1250	0.0965	0.0461	0.081*
C14	0.2385 (6)	0.0802 (8)	0.0591 (5)	0.086 (3)
H14	0.2387	-0.0065	0.0614	0.103*
C15	0.3047 (5)	0.1465 (10)	0.0636 (5)	0.085 (2)
H15	0.3529	0.1071	0.0678	0.101*
C16	0.3002 (5)	0.2702 (9)	0.0621 (5)	0.087 (3)
H16	0.3456	0.3181	0.0653	0.105*
C17	0.2305 (5)	0.3268 (8)	0.0558 (5)	0.081 (2)
H17	0.2284	0.4136	0.0559	0.097*
C18	0.2134 (4)	0.3438 (7)	-0.1238 (4)	0.0623 (19)
H18	0.2396	0.3953	-0.0983	0.075*
C19	0.2608 (5)	0.3095 (8)	-0.2012 (5)	0.079 (3)
H19	0.3180	0.3399	-0.2292	0.095*
C20	0.2249 (5)	0.2304 (8)	-0.2381 (4)	0.082 (3)
H20	0.2578	0.2018	-0.2907	0.098*
C21	0.1410 (5)	0.1944 (7)	-0.1973 (4)	0.068 (2)
H21	0.1142	0.1427	-0.2223	0.081*
C22	0.0941 (4)	0.2332 (7)	-0.1187 (4)	0.0569 (19)
H22	0.0359	0.2068	-0.0907	0.068*
C23	0.2998 (7)	0.5075 (10)	0.2214 (6)	0.109 (3)
H23	0.2847	0.4539	0.2656	0.131*
C24	0.2333 (7)	0.5803 (11)	0.2132 (7)	0.119 (3)
H24	0.1753	0.5795	0.2521	0.143*
C25	0.2579 (7)	0.6506 (11)	0.1467 (7)	0.114 (3)
H25	0.2162	0.7026	0.1401	0.137*
C26	0.3383 (7)	0.6492 (10)	0.0904 (6)	0.114 (3)
H26	0.3529	0.6934	0.0421	0.137*
C27	0.4001 (6)	0.5813 (10)	0.1043 (6)	0.103 (3)
H27	0.4583	0.5839	0.0658	0.123*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0418 (5)	0.0598 (6)	0.0440 (5)	-0.0056 (5)	-0.0140 (4)	0.0011 (5)
Co2	0.0518 (6)	0.0880 (9)	0.0837 (8)	0.0001 (6)	-0.0303 (6)	-0.0002 (6)
Cl1	0.0748 (14)	0.168 (3)	0.0835 (15)	0.0201 (15)	-0.0286 (12)	0.0046 (16)

C12	0.0994 (15)	0.0885 (17)	0.1204 (18)	0.0034 (13)	-0.0694 (14)	-0.0052 (14)
C13	0.0617 (13)	0.0981 (19)	0.160 (2)	-0.0146 (12)	-0.0280 (14)	-0.0084 (17)
N1	0.046 (3)	0.053 (4)	0.040 (3)	-0.007 (3)	-0.011 (3)	0.002 (3)
N2	0.045 (3)	0.045 (4)	0.048 (3)	-0.009 (3)	-0.016 (3)	0.003 (3)
N3	0.050 (3)	0.063 (4)	0.051 (3)	-0.007 (3)	-0.026 (3)	0.001 (3)
N4	0.037 (3)	0.058 (4)	0.050 (3)	0.000 (3)	-0.016 (3)	-0.001 (3)
N5	0.071 (5)	0.119 (7)	0.087 (5)	0.016 (4)	-0.037 (4)	-0.002 (5)
O1	0.042 (2)	0.061 (3)	0.051 (3)	-0.006 (2)	-0.018 (2)	0.006 (2)
O2	0.054 (3)	0.060 (3)	0.054 (3)	-0.009 (2)	-0.021 (2)	0.002 (2)
C1	0.038 (4)	0.067 (5)	0.035 (4)	-0.011 (4)	-0.009 (3)	0.006 (4)
C2	0.040 (4)	0.069 (5)	0.036 (4)	-0.001 (4)	-0.011 (3)	-0.003 (4)
C3	0.049 (4)	0.056 (5)	0.040 (4)	-0.020 (4)	-0.010 (3)	0.003 (4)
C4	0.067 (5)	0.067 (6)	0.080 (6)	0.003 (5)	-0.023 (4)	0.000 (5)
C5	0.077 (6)	0.079 (7)	0.102 (7)	-0.022 (5)	-0.033 (5)	0.014 (5)
C6	0.064 (5)	0.085 (6)	0.080 (6)	-0.018 (5)	-0.025 (4)	0.005 (5)
C7	0.055 (4)	0.070 (6)	0.049 (4)	0.004 (4)	-0.017 (4)	0.006 (4)
C8	0.080 (5)	0.054 (5)	0.058 (5)	-0.015 (4)	-0.022 (4)	0.003 (4)
C9	0.097 (6)	0.080 (7)	0.049 (5)	-0.015 (5)	-0.015 (4)	0.012 (5)
C10	0.108 (7)	0.090 (7)	0.052 (5)	0.013 (6)	-0.020 (5)	-0.001 (6)
C11	0.113 (7)	0.070 (6)	0.050 (5)	0.002 (5)	-0.023 (5)	-0.006 (5)
C12	0.073 (5)	0.065 (6)	0.047 (5)	-0.003 (4)	-0.015 (4)	0.002 (4)
C13	0.064 (5)	0.064 (6)	0.083 (5)	-0.012 (5)	-0.039 (4)	0.001 (5)
C14	0.096 (6)	0.059 (6)	0.124 (7)	-0.007 (5)	-0.068 (6)	0.011 (5)
C15	0.070 (5)	0.097 (7)	0.102 (6)	-0.003 (6)	-0.051 (5)	0.018 (6)
C16	0.086 (6)	0.071 (7)	0.139 (8)	-0.014 (5)	-0.081 (6)	0.015 (6)
C17	0.082 (6)	0.081 (6)	0.104 (6)	-0.008 (5)	-0.063 (5)	0.009 (5)
C18	0.043 (4)	0.084 (6)	0.056 (5)	-0.002 (4)	-0.015 (4)	-0.006 (4)
C19	0.046 (4)	0.128 (8)	0.051 (5)	-0.003 (5)	-0.007 (4)	-0.001 (5)
C20	0.066 (6)	0.125 (8)	0.040 (4)	0.015 (5)	-0.006 (4)	-0.013 (5)
C21	0.067 (5)	0.087 (6)	0.049 (5)	0.005 (4)	-0.024 (4)	-0.005 (4)
C22	0.047 (4)	0.077 (6)	0.044 (4)	-0.001 (4)	-0.016 (3)	0.004 (4)
C23	0.084 (7)	0.143 (10)	0.097 (7)	0.028 (7)	-0.033 (6)	0.003 (7)
C24	0.091 (7)	0.153 (10)	0.104 (8)	0.029 (7)	-0.030 (6)	-0.002 (8)
C25	0.095 (8)	0.138 (10)	0.108 (8)	0.036 (7)	-0.040 (7)	0.001 (8)
C26	0.095 (7)	0.142 (10)	0.104 (8)	0.021 (7)	-0.038 (7)	0.006 (7)
C27	0.082 (7)	0.126 (9)	0.102 (8)	0.020 (6)	-0.039 (6)	0.002 (7)

Geometric parameters (Å, °)

Co1—N1 ⁱ	1.848 (5)	C8—H8	0.9300
Co1—O2 ⁱ	1.853 (4)	C9—C10	1.345 (10)
Co1—O1	1.914 (4)	C9—H9	0.9300
Co1—N3	1.945 (5)	C10—C11	1.331 (10)
Co1—N2	1.960 (5)	C10—H10	0.9300
Co1—N4	1.964 (5)	C11—C12	1.368 (9)
Co2—N5	2.046 (7)	C11—H11	0.9300
Co2—C13	2.204 (2)	C12—H12	0.9300
Co2—C12	2.221 (2)	C13—C14	1.370 (9)
Co2—C11	2.230 (2)	C13—H13	0.9300

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N1—C1	1.303 (7)	C14—C15	1.334 (10)
N1—N1 ⁱ	1.368 (9)	C14—H14	0.9300
N1—Co1 ⁱ	1.848 (5)	C15—C16	1.328 (10)
N2—C12	1.306 (8)	C15—H15	0.9300
N2—C8	1.325 (8)	C16—C17	1.345 (10)
N3—C13	1.297 (8)	C16—H16	0.9300
N3—C17	1.311 (8)	C17—H17	0.9300
N4—C22	1.315 (7)	C18—C19	1.342 (9)
N4—C18	1.327 (7)	C18—H18	0.9300
N5—C23	1.297 (10)	C19—C20	1.354 (10)
N5—C27	1.308 (10)	C19—H19	0.9300
O1—C1	1.276 (7)	C20—C21	1.335 (9)
O2—C3	1.323 (7)	C20—H20	0.9300
O2—Co1 ⁱ	1.853 (4)	C21—C22	1.372 (8)
C1—C2	1.433 (9)	C21—H21	0.9300
C2—C3	1.382 (9)	C22—H22	0.9300
C2—C7	1.417 (8)	C23—C24	1.402 (12)
C3—C4	1.358 (9)	C23—H23	0.9300
C4—C5	1.373 (9)	C24—C25	1.329 (13)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.379 (10)	C25—C26	1.303 (12)
C5—H5	0.9300	C25—H25	0.9300
C6—C7	1.343 (9)	C26—C27	1.356 (12)
C6—H6	0.9300	C26—H26	0.9300
C7—H7	0.9300	C27—H27	0.9300
C8—C9	1.385 (9)		
N1 ⁱ —Co1—O2 ⁱ	92.1 (2)	N2—C8—H8	119.0
N1 ⁱ —Co1—O1	82.78 (19)	C9—C8—H8	119.0
O2 ⁱ —Co1—O1	174.87 (19)	C10—C9—C8	117.3 (8)
N1 ⁱ —Co1—N3	175.7 (2)	C10—C9—H9	121.4
O2 ⁱ —Co1—N3	91.9 (2)	C8—C9—H9	121.4
O1—Co1—N3	93.2 (2)	C11—C10—C9	121.0 (8)
N1 ⁱ —Co1—N2	92.7 (2)	C11—C10—H10	119.5
O2 ⁱ —Co1—N2	89.1 (2)	C9—C10—H10	119.5
O1—Co1—N2	91.5 (2)	C10—C11—C12	119.0 (8)
N3—Co1—N2	88.9 (2)	C10—C11—H11	120.5
N1 ⁱ —Co1—N4	91.0 (2)	C12—C11—H11	120.5
O2 ⁱ —Co1—N4	91.2 (2)	N2—C12—C11	121.9 (7)
O1—Co1—N4	88.5 (2)	N2—C12—H12	119.1
N3—Co1—N4	87.4 (2)	C11—C12—H12	119.1
N2—Co1—N4	176.3 (2)	N3—C13—C14	123.3 (7)
N5—Co2—C13	105.2 (3)	N3—C13—H13	118.4
N5—Co2—C12	108.1 (2)	C14—C13—H13	118.4
C13—Co2—C12	109.83 (10)	C15—C14—C13	118.4 (8)
N5—Co2—C11	104.9 (2)	C15—C14—H14	120.8
C13—Co2—C11	114.14 (10)	C13—C14—H14	120.8

C12—Co2—C11	114.01 (11)	C16—C15—C14	118.4 (8)
C1—N1—N1 ⁱ	113.2 (6)	C16—C15—H15	120.8
C1—N1—Co1 ⁱ	133.7 (5)	C14—C15—H15	120.8
N1 ⁱ —N1—Co1 ⁱ	112.7 (5)	C15—C16—C17	120.6 (8)
C12—N2—C8	118.7 (6)	C15—C16—H16	119.7
C12—N2—Co1	121.3 (5)	C17—C16—H16	119.7
C8—N2—Co1	119.8 (5)	N3—C17—C16	122.1 (8)
C13—N3—C17	117.2 (6)	N3—C17—H17	119.0
C13—N3—Co1	122.4 (5)	C16—C17—H17	119.0
C17—N3—Co1	120.4 (6)	N4—C18—C19	122.5 (7)
C22—N4—C18	118.3 (6)	N4—C18—H18	118.7
C22—N4—Co1	122.2 (4)	C19—C18—H18	118.7
C18—N4—Co1	119.3 (5)	C18—C19—C20	119.5 (7)
C23—N5—C27	117.6 (8)	C18—C19—H19	120.3
C23—N5—Co2	121.2 (7)	C20—C19—H19	120.3
C27—N5—Co2	120.8 (7)	C21—C20—C19	118.3 (7)
C1—O1—Co1	110.6 (4)	C21—C20—H20	120.8
C3—O2—Co1 ⁱ	125.0 (4)	C19—C20—H20	120.8
O1—C1—N1	120.2 (6)	C20—C21—C22	120.3 (7)
O1—C1—C2	121.6 (6)	C20—C21—H21	119.8
N1—C1—C2	118.2 (6)	C22—C21—H21	119.8
C3—C2—C7	119.6 (7)	N4—C22—C21	121.0 (6)
C3—C2—C1	122.5 (6)	N4—C22—H22	119.5
C7—C2—C1	117.9 (6)	C21—C22—H22	119.5
O2—C3—C4	115.0 (7)	N5—C23—C24	122.2 (10)
O2—C3—C2	127.3 (6)	N5—C23—H23	118.9
C4—C3—C2	117.7 (6)	C24—C23—H23	118.9
C3—C4—C5	122.9 (8)	C25—C24—C23	116.3 (10)
C3—C4—H4	118.6	C25—C24—H24	121.9
C5—C4—H4	118.6	C23—C24—H24	121.9
C4—C5—C6	119.6 (8)	C26—C25—C24	122.4 (10)
C4—C5—H5	120.2	C26—C25—H25	118.8
C6—C5—H5	120.2	C24—C25—H25	118.8
C7—C6—C5	119.2 (7)	C25—C26—C27	117.9 (10)
C7—C6—H6	120.4	C25—C26—H26	121.0
C5—C6—H6	120.4	C27—C26—H26	121.0
C6—C7—C2	121.0 (7)	N5—C27—C26	123.2 (9)
C6—C7—H7	119.5	N5—C27—H27	118.4
C2—C7—H7	119.5	C26—C27—H27	118.4
N2—C8—C9	122.0 (7)		

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

Table 2

C-H... π weak interaction parameters (\AA , $^\circ$)

C_g is the centroid of the C2–C7 ring.

C-H...C _g	C-H	H...C _g	C...C _g	C-H...C _g
C20-H20...C _g ⁱⁱ	0.93	2.64	3.327 (4)	132

supplementary materials

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

Fig. 1

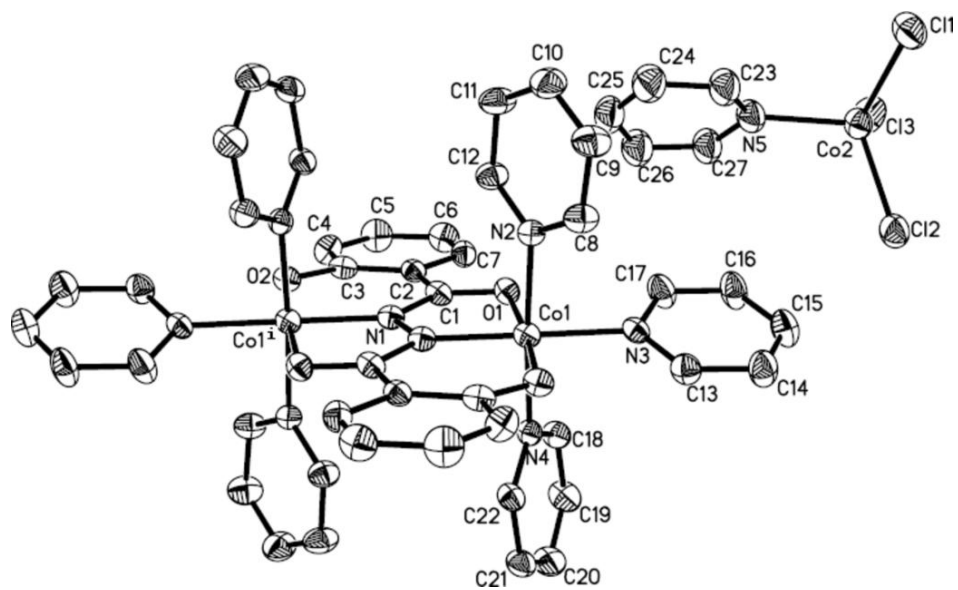


Fig. 2

