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Bis(2-aminopyridine-κN^1)bis(benzoato-κO)cobalt(II)

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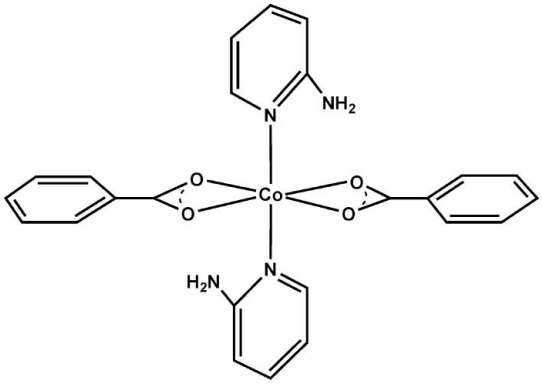
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.092; data-to-parameter ratio = 17.7.

In the title compound, $[Co(C_7H_5O_2)_2(C_5H_6N_2)_2]$, the Co^{II} atom is hexacoordinated by four O atoms from two benzoate anions, and two N atoms from two 2-aminopyridine molecules, resulting in a distorted octahedral geometry. Both benzoate anions act as bidentate ligands and both 2-aminopyridine molecules are coordinated to the metal through their pyridyl N atoms. The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds, C—H···π, and π–π stacking interactions involving benzoate anions and 2-aminopyridine molecules.

Related literature

For related literature, see: Benbellat *et al.* (2006); Brechin *et al.* (2000); Dirnitrou *et al.* (1995); Kozlevčar *et al.* (2001); Zhu, Shao *et al.* (2003); Zhu, Usman *et al.* (2003).



Experimental

Crystal data

$[Co(C_7H_5O_2)_2(C_5H_6N_2)_2]$
M_r = 489.39
Monoclinic, $P2_1/n$
a = 9.0230 (9) Å
b = 11.3787 (12) Å
c = 22.451 (2) Å
β = 96.7650 (10)°
V = 2288.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 296 (2) K
0.36 × 0.28 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.770, T_{max} = 0.835
19674 measured reflections
5288 independent reflections
4198 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.05
5288 reflections
298 parameters
357 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O4	2.0364 (15)	Co1—O1	2.1426 (18)
Co1—N3	2.1033 (16)	Co1—O2	2.2340 (17)
Co1—N1	2.1050 (16)	Co1—O3	2.4016 (17)
O4—Co1—N3	102.55 (6)	N1—Co1—O2	153.21 (7)
O4—Co1—N1	100.77 (7)	O1—Co1—O2	59.31 (6)
N3—Co1—N1	99.40 (6)	O4—Co1—O3	57.88 (5)
N3—Co1—O1	95.25 (7)	N3—Co1—O3	160.43 (6)
N1—Co1—O1	100.34 (6)	N1—Co1—O3	85.79 (6)
O4—Co1—O2	93.20 (7)	O1—Co1—O3	102.40 (6)
N3—Co1—O2	99.72 (7)	O2—Co1—O3	82.44 (6)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	2.03	2.866 (2)	163
N2—H2B···O3^{i}	0.86	2.07	2.891 (2)	158
N4—H4A···O4	0.86	1.99	2.810 (2)	160
N4—H4B···O2^{ii}	0.86	2.14	2.980 (2)	167
C13—H13···$Cg1^{iii}$	0.93	2.95	3.719 (3)	141

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, 1-y, -z$. $Cg1$ is the centroid of the N1/C20–C24 ring.

Table 3
π–π Interactions (Å, °).

π–π Contacts	Cg···Cg	α^a	β^b	Cg···Plane
Cg(N3→C19)···Cg(C2→C7)^{iv}	3.7145 (16)	6.3	16.0	3.535
Cg(C2→C7)···Cg(N3→C19)^{v}	3.7145 (16)	6.3	17.9	3.570

Notes: α^a = angle between planes of two aromatic rings. β^b = angle between Cg···Cg line and normal to the plane of the first aromatic ring. Symmetry codes: (iv) $-1+x, y, z$; (v) $1+x, y, z$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: KP2149).

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supplementary materials

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Bis(2-aminopyridine-κN^1)bis(benzoato-κO)cobalt(II)

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Comment

In recent years the study of crystal structures and properties of cobalt complexes based on carboxyl ligand, owing to their novel geometries and magnetic behaviours, have attracted chemists (Tan *et al.*, 2003; Zheng *et al.*, 2004; Wang *et al.*, 2004; Shi *et al.*, 2004) to explore their use. The structures of the mixed ligand complexes containing benzoate as the most simple aromatic carboxyl compoud with well antibacterial activity and 2-aminopyridine reported by (Kozlevčar *et al.*, 2001; Zhu, Usman *et al.*, 2003; Zhu, Shao *et al.*, 2004). Herein, we report the synthesis and crystal structure of mixed ligands cobalt(II) complex.

The stucture of the title compound (I) is isostructural with the nickel (**I**) complex (Zhu, Shao *et al.*, 2003) with the Co^{II} atom hexa-coordinated by four O atoms of two benzoato anions, and two independent pyridine N atoms from two 2-aminopyridine molecules in distorted octahedral geometry (Fig. 1). The Co—N bond lengths of 2.1030 (14) Å and 2.1054 (14) Å, the Co—O distances ranging from 2.0363 (13) to 2.4016 (15) Å, are in the normal range. The close carboxylato distances O1—C8 and O2—C8, 1.260 (2) Å and 1.250 (2) Å, O3—C1 and O4—C1, 1.241 (2) Å and 1.274 (2) Å reveal the bidentate benzoato function. The molecules are held together by intramolecular and intermolecular hydrogen bonds, C—H···π and π–π stacking interactions generating three-dimensional supramolecular network.The amide N2 and N4 donate H atoms to the carboxyl O atoms O1and O4 in intramolecular N2—H2A···O1 and N4—H4A···O4 hydrogen bonds. The N2 and N4 also donate H atoms to O2 and O3 to form intermolecular N2—H2B···O2 and N4—H4B···O3 hydrogen bonds. Intermolecular C—H···π interation is pronounced in this crystal structure involving methyl group C13 of the benzoato and the pyridyl rings N1→C24, with the distance 2.95 Å between the methyl hydrogen and the centroid of the nearest aromatic ring. In addition, π–π stacking interactions are also observed; the distance between centroids of the pyridyl ring N3→C19 and the aromatic ring C2→C7 is 3.7145 (16) Å (Table 1, Fig. 2).

Experimental

The reagents available commercially were used without further purification. $Co(NO_3)_2.6H_2O$ (0.5 mmol), benzoate sodium (1 mmol) and 2-aminopyridine (1 mmol) were mixed in solution containing 8 ml of ethanol and 8 ml of water. After stirring 1.5 h, the mixture was placed in 25 ml Teflon-lined reactor and heated at 383 K in an oven for 7 days. The resulting solution was filtered and the filtrate was allowed to stay at ambience temperature. Well shaped purple crystals suitable for X-rays diffraction were obtained after two weeks. Yield: 78%.

Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H, C—H distances of 0.86 Å, 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C or N).

Figures

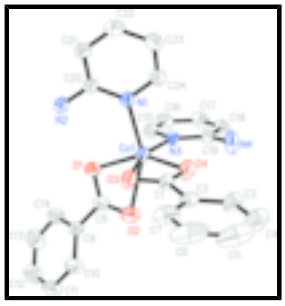


Fig. 1. The structure of (**I**) with the 30% probability displacement ellipsoids and the atom-labeling scheme.

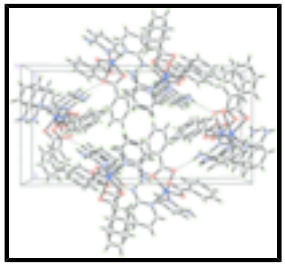


Fig. 2. Three-dimensional supramolecular network constructed by hydrogen bonding (dashed lines) and C—H···π, π-π interactions.

Bis(2-aminopyridine-κ*N*^{1})bis(benzoato-κ*O*)cobalt(II)

Crystal data

$[Co(C_7H_5O_2)_2(C_5H_6N_2)_2]$	F_{000} = 1012
M_r = 489.39	D_x = 1.420 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7256 reflections
a = 9.0230 (9) Å	θ = 2.4–27.2º
b = 11.3787 (12) Å	μ = 0.79 mm^{-1}
c = 22.451 (2) Å	T = 296 (2) K
β = 96.7650 (10)º	Block, purple
V = 2288.9 (4) Å^3	0.36 × 0.28 × 0.22 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	5288 independent reflections
Radiation source: fine-focus sealed tube	4198 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
T = 296(2) K	θ_{max} = 27.7º
phi and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.770, T_{max} = 0.835	k = −14→14
19674 measured reflections	l = −29→25

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.6259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.050$
5288 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
357 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.29899 (3)	0.42895 (2)	0.123207 (11)	0.04251 (10)
N1	0.37446 (18)	0.31734 (14)	0.05834 (7)	0.0434 (4)
N2	0.3314 (2)	0.44408 (15)	−0.02241 (8)	0.0520 (4)
H2A	0.2773	0.4869	−0.0019	0.062*
H2B	0.3439	0.4640	−0.0584	0.062*
N3	0.11106 (18)	0.33308 (14)	0.14242 (7)	0.0429 (4)
N4	0.2282 (2)	0.2407 (2)	0.22706 (9)	0.0745 (6)
H4A	0.3108	0.2736	0.2208	0.089*
H4B	0.2254	0.1949	0.2574	0.089*
O1	0.1750 (2)	0.55468 (13)	0.06636 (7)	0.0651 (5)
O2	0.2427 (2)	0.60479 (15)	0.15868 (8)	0.0698 (5)
O3	0.54634 (19)	0.51020 (15)	0.13357 (6)	0.0602 (4)
O4	0.45109 (17)	0.39318 (15)	0.19532 (6)	0.0566 (4)
C1	0.5594 (2)	0.45573 (18)	0.18175 (9)	0.0444 (4)
C2	0.6981 (2)	0.4610 (2)	0.22510 (10)	0.0504 (5)
C3	0.7083 (3)	0.3990 (3)	0.27797 (11)	0.0690 (7)
H3	0.6284	0.3539	0.2875	0.083*

C4	0.8401 (4)	0.4045 (3)	0.31715 (15)	0.0957 (10)
H4	0.8483	0.3637	0.3533	0.115*
C5	0.9565 (4)	0.4697 (4)	0.30237 (19)	0.1039 (11)
H5	1.0446	0.4716	0.3284	0.125*
C6	0.9476 (3)	0.5316 (4)	0.2510 (2)	0.1015 (11)
H6	1.0283	0.5765	0.2421	0.122*
C7	0.8173 (3)	0.5283 (3)	0.21134 (14)	0.0760 (7)
H7	0.8102	0.5710	0.1758	0.091*
C8	0.1784 (2)	0.62950 (18)	0.10788 (10)	0.0520 (5)
C9	0.1044 (2)	0.74580 (18)	0.09538 (10)	0.0499 (5)
C10	0.1555 (3)	0.8438 (2)	0.12792 (12)	0.0667 (6)
H10	0.2364	0.8373	0.1575	0.080*
C11	0.0872 (4)	0.9512 (2)	0.11675 (15)	0.0842 (8)
H11	0.1236	1.0173	0.1381	0.101*
C12	−0.0346 (4)	0.9607 (3)	0.07410 (16)	0.0886 (9)
H12	−0.0813	1.0331	0.0670	0.106*
C13	−0.0872 (4)	0.8644 (3)	0.04219 (15)	0.0880 (8)
H13	−0.1706	0.8709	0.0138	0.106*
C14	−0.0171 (3)	0.7572 (2)	0.05190 (12)	0.0696 (7)
H14	−0.0515	0.6923	0.0292	0.084*
C15	−0.0147 (2)	0.3464 (2)	0.10357 (10)	0.0529 (5)
H15	−0.0106	0.3956	0.0707	0.063*
C16	−0.1465 (3)	0.2924 (2)	0.10970 (12)	0.0634 (6)
H16	−0.2295	0.3033	0.0815	0.076*
C17	−0.1537 (3)	0.2207 (2)	0.15906 (12)	0.0643 (6)
H17	−0.2426	0.1834	0.1648	0.077*
C18	−0.0309 (3)	0.2052 (2)	0.19887 (11)	0.0594 (6)
H18	−0.0353	0.1578	0.2324	0.071*
C19	0.1036 (2)	0.26105 (18)	0.18948 (9)	0.0479 (5)
C20	0.3961 (2)	0.34636 (17)	0.00178 (8)	0.0426 (4)
C21	0.4848 (3)	0.27532 (19)	−0.03144 (10)	0.0532 (5)
H21	0.5028	0.2980	−0.0697	0.064*
C22	0.5438 (3)	0.1739 (2)	−0.00744 (11)	0.0610 (6)
H22	0.6025	0.1268	−0.0291	0.073*
C23	0.5157 (3)	0.1407 (2)	0.05002 (11)	0.0614 (6)
H23	0.5525	0.0704	0.0669	0.074*
C24	0.4331 (3)	0.21426 (19)	0.08048 (10)	0.0548 (5)
H24	0.4156	0.1926	0.1190	0.066*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.04193 (16)	0.05067 (17)	0.03496 (15)	−0.00377 (11)	0.00463 (10)	0.00284 (11)
N1	0.0453 (9)	0.0461 (9)	0.0388 (8)	−0.0058 (7)	0.0051 (7)	0.0010 (7)
N2	0.0644 (11)	0.0542 (10)	0.0393 (9)	0.0026 (8)	0.0141 (8)	0.0041 (7)
N3	0.0430 (9)	0.0459 (9)	0.0404 (8)	−0.0037 (7)	0.0080 (7)	−0.0016 (7)
N4	0.0630 (13)	0.0910 (16)	0.0676 (13)	−0.0130 (11)	0.0000 (10)	0.0383 (12)
O1	0.0964 (13)	0.0450 (8)	0.0594 (10)	−0.0035 (8)	0.0324 (9)	−0.0087 (7)

O2	0.0713 (11)	0.0598 (10)	0.0745 (11)	0.0096 (8)	−0.0071 (9)	−0.0133 (9)
O3	0.0701 (10)	0.0665 (10)	0.0455 (8)	−0.0001 (8)	0.0132 (7)	0.0081 (7)
O4	0.0462 (8)	0.0740 (10)	0.0483 (8)	−0.0136 (7)	0.0003 (6)	0.0080 (7)
C1	0.0448 (11)	0.0493 (10)	0.0399 (10)	0.0008 (8)	0.0088 (8)	−0.0041 (8)
C2	0.0403 (10)	0.0578 (12)	0.0537 (12)	0.0024 (9)	0.0082 (9)	−0.0181 (10)
C3	0.0601 (14)	0.0847 (16)	0.0591 (14)	0.0156 (12)	−0.0058 (11)	−0.0075 (12)
C4	0.083 (2)	0.119 (2)	0.0781 (18)	0.0320 (18)	−0.0214 (16)	−0.0218 (17)
C5	0.0558 (17)	0.136 (3)	0.113 (2)	0.0282 (18)	−0.0207 (17)	−0.062 (2)
C6	0.0519 (15)	0.125 (2)	0.128 (3)	−0.0153 (16)	0.0137 (17)	−0.060 (2)
C7	0.0550 (14)	0.0890 (17)	0.0862 (17)	−0.0142 (13)	0.0174 (13)	−0.0327 (15)
C8	0.0520 (12)	0.0452 (11)	0.0625 (13)	−0.0078 (9)	0.0225 (10)	−0.0096 (10)
C9	0.0507 (12)	0.0462 (10)	0.0556 (12)	−0.0041 (9)	0.0179 (9)	−0.0073 (9)
C10	0.0746 (16)	0.0515 (12)	0.0732 (15)	−0.0025 (11)	0.0052 (12)	−0.0129 (11)
C11	0.108 (2)	0.0492 (13)	0.097 (2)	0.0020 (14)	0.0172 (18)	−0.0177 (13)
C12	0.098 (2)	0.0639 (16)	0.106 (2)	0.0221 (15)	0.0193 (18)	0.0063 (16)
C13	0.0807 (19)	0.0802 (19)	0.100 (2)	0.0087 (15)	−0.0046 (16)	0.0101 (16)
C14	0.0707 (16)	0.0606 (14)	0.0754 (16)	−0.0063 (12)	−0.0003 (13)	−0.0067 (12)
C15	0.0504 (12)	0.0540 (12)	0.0530 (12)	−0.0063 (9)	0.0013 (9)	0.0007 (10)
C16	0.0467 (12)	0.0608 (13)	0.0809 (16)	−0.0081 (10)	−0.0001 (11)	−0.0041 (12)
C17	0.0498 (13)	0.0555 (13)	0.0900 (17)	−0.0121 (10)	0.0191 (12)	−0.0067 (12)
C18	0.0655 (14)	0.0483 (11)	0.0686 (14)	−0.0083 (10)	0.0257 (12)	0.0039 (10)
C19	0.0511 (11)	0.0451 (10)	0.0495 (11)	−0.0017 (9)	0.0146 (9)	−0.0001 (9)
C20	0.0412 (10)	0.0454 (10)	0.0412 (9)	−0.0104 (8)	0.0050 (8)	−0.0040 (8)
C21	0.0579 (13)	0.0544 (12)	0.0493 (11)	−0.0079 (10)	0.0151 (9)	−0.0079 (9)
C22	0.0602 (14)	0.0558 (13)	0.0685 (14)	−0.0024 (10)	0.0141 (11)	−0.0156 (11)
C23	0.0654 (14)	0.0489 (12)	0.0683 (14)	0.0016 (10)	0.0015 (11)	−0.0004 (11)
C24	0.0614 (13)	0.0525 (12)	0.0503 (12)	−0.0043 (10)	0.0058 (10)	0.0039 (10)

Geometric parameters (Å, °)

Co1—O4	2.0364 (15)	C6—H6	0.9300
Co1—N3	2.1033 (16)	C7—H7	0.9300
Co1—N1	2.1050 (16)	C8—C9	1.494 (3)
Co1—O1	2.1426 (18)	C9—C10	1.383 (3)
Co1—O2	2.2340 (17)	C9—C14	1.386 (3)
Co1—O3	2.4016 (17)	C10—C11	1.378 (4)
N1—C20	1.348 (2)	C10—H10	0.9300
N1—C24	1.357 (3)	C11—C12	1.374 (4)
N2—C20	1.341 (3)	C11—H11	0.9300
N2—H2A	0.8600	C12—C13	1.364 (5)
N2—H2B	0.8600	C12—H12	0.9300
N3—C19	1.345 (3)	C13—C14	1.379 (4)
N3—C15	1.356 (3)	C13—H13	0.9300
N4—C19	1.344 (3)	C14—H14	0.9300
N4—H4A	0.8600	C15—C16	1.360 (3)
N4—H4B	0.8600	C15—H15	0.9300
O1—C8	1.260 (3)	C16—C17	1.384 (4)
O2—C8	1.249 (3)	C16—H16	0.9300
O3—C1	1.240 (2)	C17—C18	1.350 (4)

O4—C1	1.274 (2)	C17—H17	0.9300
C1—C2	1.493 (3)	C18—C19	1.408 (3)
C2—C3	1.375 (3)	C18—H18	0.9300
C2—C7	1.385 (3)	C20—C21	1.411 (3)
C3—C4	1.395 (4)	C21—C22	1.355 (3)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.359 (6)	C22—C23	1.396 (3)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.345 (5)	C23—C24	1.358 (3)
C5—H5	0.9300	C23—H23	0.9300
C6—C7	1.389 (4)	C24—H24	0.9300
O4—Co1—N3	102.55 (6)	O2—C8—O1	119.5 (2)
O4—Co1—N1	100.77 (7)	O2—C8—C9	121.34 (19)
N3—Co1—N1	99.40 (6)	O1—C8—C9	119.2 (2)
O4—Co1—O1	149.63 (7)	C10—C9—C14	118.9 (2)
N3—Co1—O1	95.25 (7)	C10—C9—C8	120.1 (2)
N1—Co1—O1	100.34 (6)	C14—C9—C8	121.0 (2)
O4—Co1—O2	93.20 (7)	C11—C10—C9	120.3 (3)
N3—Co1—O2	99.72 (7)	C11—C10—H10	119.8
N1—Co1—O2	153.21 (7)	C9—C10—H10	119.8
O1—Co1—O2	59.31 (6)	C12—C11—C10	120.1 (3)
O4—Co1—O3	57.88 (5)	C12—C11—H11	120.0
N3—Co1—O3	160.43 (6)	C10—C11—H11	120.0
N1—Co1—O3	85.79 (6)	C13—C12—C11	120.2 (3)
O1—Co1—O3	102.40 (6)	C13—C12—H12	119.9
O2—Co1—O3	82.44 (6)	C11—C12—H12	119.9
C20—N1—C24	117.60 (18)	C12—C13—C14	120.2 (3)
C20—N1—Co1	126.75 (13)	C12—C13—H13	119.9
C24—N1—Co1	114.33 (13)	C14—C13—H13	119.9
C20—N2—H2A	120.0	C13—C14—C9	120.3 (3)
C20—N2—H2B	120.0	C13—C14—H14	119.8
H2A—N2—H2B	120.0	C9—C14—H14	119.8
C19—N3—C15	117.26 (17)	N3—C15—C16	124.0 (2)
C19—N3—Co1	126.38 (14)	N3—C15—H15	118.0
C15—N3—Co1	116.35 (13)	C16—C15—H15	118.0
C19—N4—H4A	120.0	C15—C16—C17	118.2 (2)
C19—N4—H4B	120.0	C15—C16—H16	120.9
H4A—N4—H4B	120.0	C17—C16—H16	120.9
C8—O1—Co1	92.57 (15)	C18—C17—C16	119.7 (2)
C8—O2—Co1	88.66 (13)	C18—C17—H17	120.2
C1—O3—Co1	83.32 (13)	C16—C17—H17	120.2
C1—O4—Co1	99.33 (12)	C17—C18—C19	119.8 (2)
O3—C1—O4	119.41 (19)	C17—C18—H18	120.1
O3—C1—C2	122.31 (19)	C19—C18—H18	120.1
O4—C1—C2	118.28 (18)	N4—C19—N3	118.84 (18)
C3—C2—C7	120.1 (2)	N4—C19—C18	120.1 (2)
C3—C2—C1	120.5 (2)	N3—C19—C18	121.1 (2)
C7—C2—C1	119.4 (2)	N2—C20—N1	118.69 (18)
C2—C3—C4	119.1 (3)	N2—C20—C21	120.54 (18)

C2—C3—H3	120.4	N1—C20—C21	120.77 (19)
C4—C3—H3	120.4	C22—C21—C20	119.9 (2)
C5—C4—C3	119.8 (4)	C22—C21—H21	120.1
C5—C4—H4	120.1	C20—C21—H21	120.1
C3—C4—H4	120.1	C21—C22—C23	119.5 (2)
C4—C5—C6	121.7 (3)	C21—C22—H22	120.3
C4—C5—H5	119.1	C23—C22—H22	120.3
C6—C5—H5	119.2	C24—C23—C22	118.0 (2)
C5—C6—C7	119.7 (3)	C24—C23—H23	121.0
C5—C6—H6	120.1	C22—C23—H23	121.0
C7—C6—H6	120.1	C23—C24—N1	124.2 (2)
C2—C7—C6	119.5 (3)	C23—C24—H24	117.9
C2—C7—H7	120.2	N1—C24—H24	117.9
C6—C7—H7	120.2		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1	0.86	2.03	2.866 (2)	163
N2—H2B···O3^{i}	0.86	2.07	2.891 (2)	158
N4—H4A···O4	0.86	1.99	2.810 (2)	160
N4—H4B···O2^{ii}	0.86	2.14	2.980 (2)	167

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1/2, *y*−1/2, −*z*+1/2.

Table 3

C-H···π interactions (Å, °)

C—H···Cg^{a}	H···Cg	C···Cg	γ^{b}	C—H···Cg
C13—H13···Cg(N1→C24)^{iii}	2.95	3.719 (3)	6.07	141

Notes: Cg^{a} = centre of gravity of the six-membered ring. γ^{b} = angle defined by a line connecting centre of gravity of the six-membered ring with H atom and the normal to the six-membered ring. Symmetry code: (iii) -*x*, 1 - *y*, -*z*.

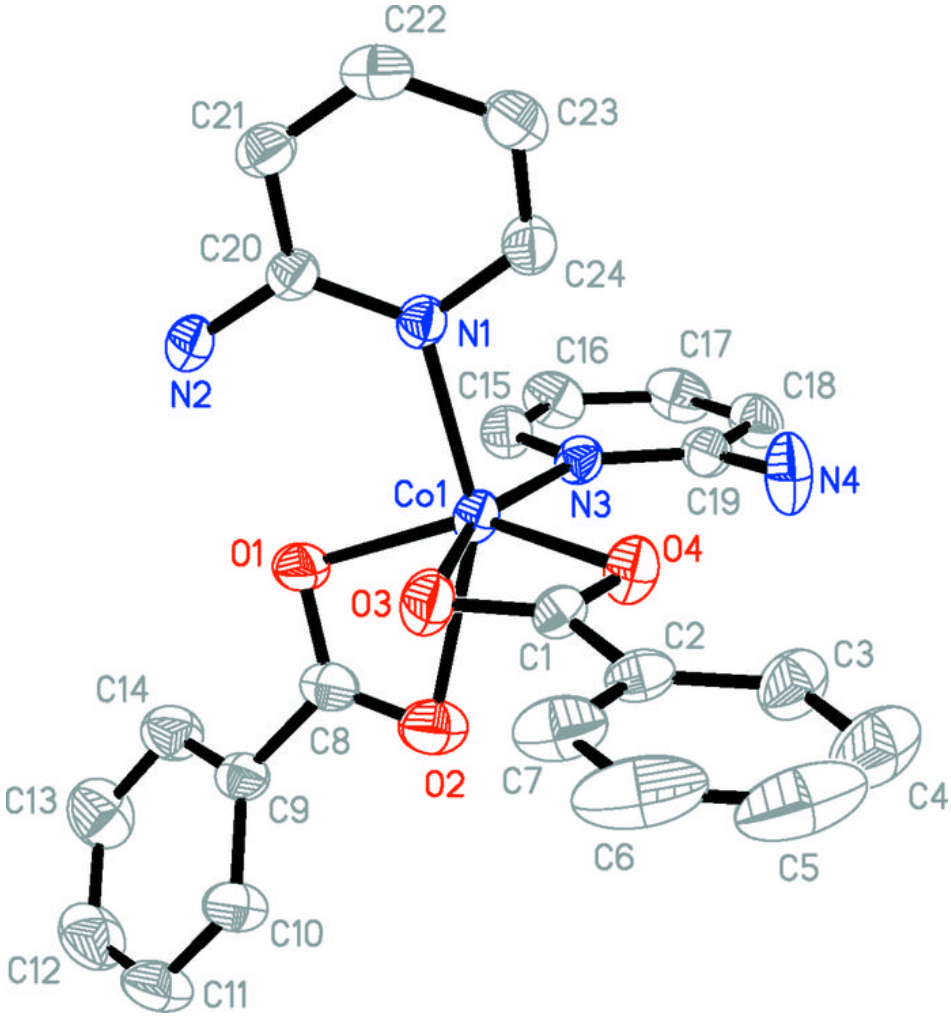
Table 4

π–π interactions (Å, °)

π–π contacts	Cg···Cg	α^{a}(	β^{b}	Cg···Plane
Cg(N3→C19)···Cg(C2→C7)^{iv}	3.7145 (16)	6.30	16.02	3.535
Cg(C2→C7)···Cg(N3→C19)^{v}	3.7145 (16)	6.30	17.87	3.570

Notes: α^{a} = angle between planes of two aromatic rings. β^{b} = angle between Cg···Cg line and normal to the plane of the first aromatic ring. Symmetry codes: (iv) -1 + *x*, *y*, *z*; (v) 1 + *x*, *y*, *z*.

Fig. 1


C22
C21
C23
C20
C24
N1
N2
C16
C17
C15
C18
N3
C19
N4
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O1
O4
O3
C1
C2
C3
C14
C8
O2
C7
C4
C13
C9
C6
C5
C10
C12
C11

Fig. 2