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Bis[2-(benzimidazol-2-yl)phenolato-κ^2N,O]cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.044
wR factor = 0.114
Data-to-parameter ratio = 17.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Co(C_{13}H_9N_2O)_2]$, the coordination geometry of the Co^{II} atom is distorted tetrahedral; the Co atom lies on a twofold axis. Adjacent molecules are linked by N—H···O hydrogen bonds into a three-dimensional network structure.

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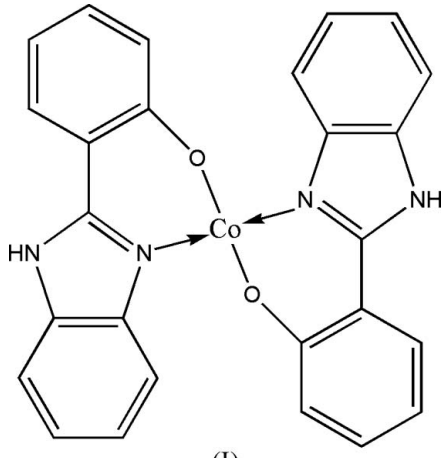
Comment

2-(Benzimidazol-2-yl)phenol is a bidentate heterocycle that possesses a benzimidazole nitrogen and a phenol oxygen site; it also has an additional hydrogen-bond donor unit (NH) (Crane *et al.*, 1995).



(I)

In the structure of (I), the Co^{II} atom lies on a twofold axis and is coordinated by two N atoms and two O atoms to give a distorted tetrahedral geometry (Fig. 1). The benzimidazole and phenol groups are nearly coplanar; the dihedral angle between them is 3.6 (2)°. The angle between the two ligand planes is 83.10 (5)°. The complexes are linked by N—H···O hydrogen bonds [N···O = 2.809 (3) Å and N—H···O = 144°] into a three-dimensional network structure.

Experimental

Cobalt nitrate hexahydrate (0.146 g, 0.5 mmol) and 2-(benzimidazol-2-yl)phenol (0.210 g, 1 mmol) were dissolved in ethanol (3 ml) and water (15 ml). The solution was placed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated at 433 K for 120 h. The cooled mixture yielded red crystals of (I); these were washed with water and then dried in air (yield *ca* 70%).

Crystal data

$[Co(C_{13}H_9N_2O)_2]$
M_r = 477.37
Tetragonal, $P4_12_12$
a = 9.9452 (3) Å
c = 22.581 (2) Å
V = 2233.4 (2) Å^3
Z = 4
D_x = 1.420 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1671 reflections
θ = 3.0–25.4°
μ = 0.80 mm^{-1}
T = 293 (2) K
Block, red
0.17 × 0.15 × 0.14 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.876, T_{max} = 0.896
15456 measured reflections
2669 independent reflections
2346 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 28.3°
$h = -12 \rightarrow 13$
$k = -12 \rightarrow 10$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.09
2669 reflections
150 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.7603P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 986 Friedel pairs
Flack parameter: 0.49 (3)

Table 1
Selected geometric parameters (Å, °).

Co1—O1	1.912 (2)	Co1—N2	1.950 (2)
O1^i—Co1—O1	120.25 (13)	O1^i—Co1—N2	112.81 (9)
O1—Co1—N2	94.22 (9)	N2—Co1—N2^i	124.83 (15)

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

The crystal is a racemic twin, can be refined in $P4_12_12$ with a Flack (1983) parameter of 0.49 (3) and in $P4_32_12$ with a Flack parameter of 0.52 (2). All H atoms were positioned geometrically and refined using a riding model, with distances C—H = 0.93 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2005); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2005); software used to prepare material for publication: *SHELXTL*.

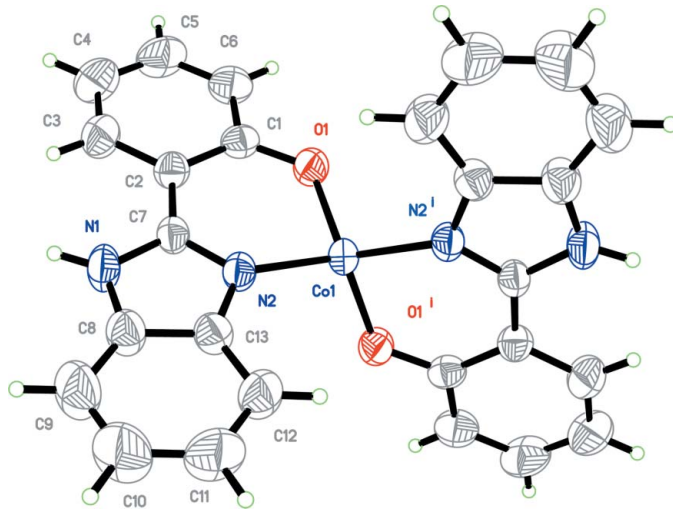


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms as spheres of arbitrary radii. [symmetry code: (i) $y, x, -z$].

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