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Poly[(3-nitrobenzoato)(μ_3-1,2,4-triazolato)cobalt(II)]

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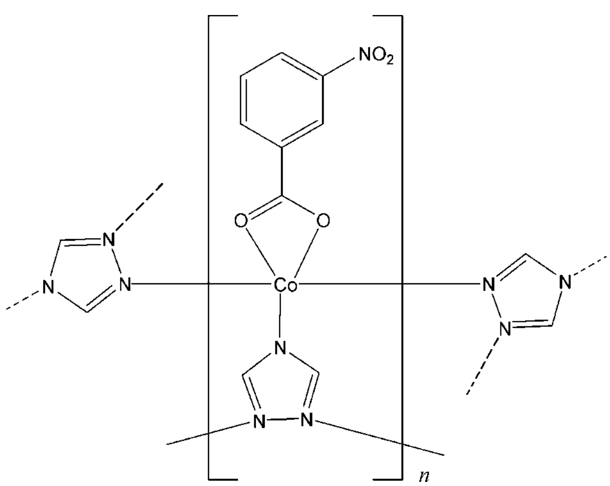
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.023; wR factor = 0.059; data-to-parameter ratio = 15.2.

In the title compound, $[Co(C_2H_2N_3)(C_7H_4NO_4)]_n$, the Co^{II} atom is five-coordinated by three triazolate ligands and one bidentate 3-nitrobenzoate anion in a distorted trigonal-bipyramidal geometry. The triazolate ligand bridges the Co^{II} atoms, generating a two-dimensional net parallel to the ab plane, in which both the Co^{II} atom and the triazolate ligand act as three-connected nodes. Two weak intermolecular C—H···O hydrogen bonds connect the nets.

Related literature

For metal–triazole complexes, see: Park *et al.* (2006); Yang *et al.* (2008); Zhai *et al.* (2007). For Co—O and Co—N bond lengths, see: Zhang *et al.* (2008).



Experimental

Crystal data

$[Co(C_2H_2N_3)(C_7H_4NO_4)]$
M_r = 293.11
Orthorhombic, $Pbca$
a = 9.2419 (18) Å
b = 10.377 (2) Å
c = 22.597 (5) Å
V = 2167.1 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.60 mm^{-1}
T = 296 (2) K
0.14 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.802, T_{max} = 0.826
19233 measured reflections
2477 independent reflections
2245 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.059
S = 1.04
2477 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.3314 (12)	Co1—N2^{i}	2.0118 (12)
Co1—O2	2.0008 (12)	Co1—N3^{ii}	2.0385 (12)
Co1—N1	2.0232 (12)		

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (ii) $-x + \frac{1}{2}, y - \frac{1}{2}, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{iii}	0.93	2.54	3.250 (3)	134
C8—H8···O4^{iv}	0.93	2.46	3.372 (2)	169

Symmetry codes: (iii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2370).

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supplementary materials

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Poly[(3-nitrobenzoato)(μ_3-1,2,4-triazolato)cobalt(II)]

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Comment

Recently, more and more attention is paid on the coordination chemistry about trz ligand or analogy ligand (Park *et al.*, 2006; Yang *et al.*, 2008; Zhai *et al.*, 2007), driven by their intriguing topological matrix and potential applications.

The asymmetric unit of I is shown in Fig. 1. The Co^{II} atom is five-coordinated by two *L* (3-nitrobenzoate anion) O atoms, three trz N atoms to give rise to a distorted trigonal-bipyramidal geometry. The Co—O/N bond lengths of 2.0008 (12)–2.3314 (12)Å (Table 1) are in the normal range (Zhang *et al.*, 2008). The trz and *L* ligand adopt bridging and bidentate coordinated modes, respectively. As shown in Fig. 2a, the Co^{II} atoms are combined together by trz ligands to generate a two-dimensional net parallel to the *ab* plane with the *L* ligands ligated on the two-dimensional net up and down. From a topological point of view, if considering the trz ligands and cobalt ions as three-connected nodes. Moreover, besides the presence of two weak intermolecular C—H···O hydrogen bonds, see Table 2, there is not other obvious supramolecular interactions between two-dimensional nets,

Experimental

$CoCl_2$ (1.0 mmol), 3-nitrobenzoic acid (1 mmol) and triazole (1 mmol) were dissolved in water (10 ml). The solution was heated in a 25 ml Teflonlined reaction vessel at 433 K for *ca* 3 days and then cooled to room temperature. Purple crystals of the title compound were obtained in a yield of 78%.

Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

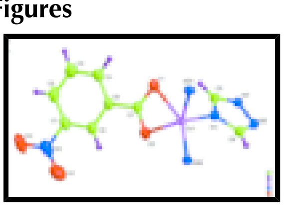

Fig. 1. An *ORTEP* view of the asymmetric unit with 50% thermal ellipsoids for non-H atoms [symmetry codes: (A) -*x* + 1/2, *y* - 1/2, *z*; (B) *x* + 1/2, -*y* + 3/2, -*z* + 1].

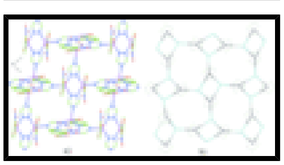

Fig. 2. a) View of the two-dimensional net onto the *ab* plane, formed by cobalt ions and trz ligands; b) View of the two-dimensional net built on three-connected trz and cobalt nodes.

Poly[(3-nitrobenzoato)(μ_3-1,2,4-triazolato)cobalt(II)]

Crystal data

$[Co(C_2H_2N_3)(C_7H_4NO_4)]$	$F_{000} = 1176$
$M_r = 293.11$	$D_x = 1.797$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 15896 reflections
a = 9.2419 (18) Å	θ = 3.1–27.5º
b = 10.377 (2) Å	μ = 1.60 mm^{-1}
c = 22.597 (5) Å	*T* = 296 (2) K
V = 2167.1 (8) Å^3	Block, purple
Z = 8	0.14 × 0.12 × 0.12 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2477 independent reflections
Radiation source: sealed tube	2245 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
Detector resolution: 8.192 pixels mm^{-1}	$\theta_{max} = 27.5$º
T = 296(2) K	$\theta_{min} = 3.1$º
ω scans	$h = -12 \rightarrow 11$
Absorption correction: Multi-scan (*SADABS*; Sheldrick, 2004)	$k = -13 \rightarrow 12$
$T_{min} = 0.802$, $T_{max} = 0.826$	$l = -29 \rightarrow 29$
19233 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.023$	H-atom parameters constrained
$wR(F^2) = 0.059$	$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.1998P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} = 0.001$
2477 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$

C1	0.0918 (2)	0.62096 (17)	0.17212 (8)	0.0358 (4)
C2	−0.0058 (2)	0.7078 (2)	0.14920 (8)	0.0470 (5)
H2	−0.0198	0.7141	0.1085	0.056*
C3	−0.0823 (3)	0.7853 (2)	0.18746 (9)	0.0522 (6)
H3	−0.1473	0.8457	0.1728	0.063*
C4	−0.0620 (2)	0.77306 (18)	0.24798 (8)	0.0406 (4)
H4	−0.1157	0.8240	0.2738	0.049*
C5	0.1165 (2)	0.60861 (16)	0.23241 (7)	0.0322 (4)
H5	0.1843	0.5503	0.2468	0.039*
C6	0.03721 (19)	0.68583 (16)	0.27043 (7)	0.0295 (3)
C7	0.05354 (18)	0.67429 (16)	0.33614 (7)	0.0290 (3)
C8	0.32376 (16)	0.75394 (14)	0.51070 (7)	0.0253 (3)
H8	0.3425	0.6826	0.5344	0.030*
C9	0.22994 (17)	0.87843 (13)	0.44808 (6)	0.0231 (3)
H9	0.1693	0.9118	0.4190	0.028*
Co1	0.08538 (2)	0.615646 (17)	0.442261 (8)	0.01829 (7)
N1	0.21652 (13)	0.75890 (11)	0.47077 (5)	0.0227 (2)
N2	0.39953 (13)	0.86141 (12)	0.51260 (5)	0.0225 (3)
N3	0.33828 (13)	0.94272 (11)	0.47154 (5)	0.0209 (2)
N4	0.1706 (2)	0.53740 (17)	0.13114 (7)	0.0459 (4)
O1	−0.00457 (13)	0.75383 (12)	0.36970 (5)	0.0367 (3)
O2	0.12664 (15)	0.58069 (12)	0.35684 (5)	0.0351 (3)
O3	0.2746 (2)	0.47839 (18)	0.14938 (7)	0.0683 (5)
O4	0.1257 (2)	0.53020 (16)	0.08006 (6)	0.0627 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0517 (11)	0.0329 (9)	0.0228 (8)	−0.0083 (7)	0.0032 (7)	−0.0016 (6)
C2	0.0745 (14)	0.0453 (11)	0.0211 (8)	−0.0027 (10)	−0.0091 (8)	0.0050 (8)
C3	0.0778 (16)	0.0444 (12)	0.0345 (10)	0.0148 (10)	−0.0150 (9)	0.0058 (9)
C4	0.0592 (11)	0.0331 (9)	0.0295 (9)	0.0079 (8)	−0.0040 (8)	0.0000 (7)
C5	0.0422 (9)	0.0299 (8)	0.0246 (8)	−0.0020 (7)	−0.0011 (7)	0.0013 (6)
C6	0.0418 (9)	0.0261 (8)	0.0208 (7)	−0.0037 (7)	−0.0026 (6)	0.0022 (6)
C7	0.0371 (8)	0.0284 (8)	0.0214 (7)	−0.0058 (6)	−0.0020 (6)	0.0014 (6)
C8	0.0290 (7)	0.0196 (7)	0.0274 (7)	−0.0033 (6)	−0.0042 (6)	0.0061 (6)
C9	0.0269 (7)	0.0190 (7)	0.0234 (7)	−0.0015 (5)	−0.0031 (5)	0.0034 (5)
Co1	0.02203 (12)	0.01445 (11)	0.01838 (11)	−0.00039 (6)	0.00086 (7)	0.00145 (7)
N1	0.0263 (6)	0.0181 (6)	0.0238 (6)	−0.0032 (5)	−0.0026 (5)	0.0025 (5)
N2	0.0247 (6)	0.0185 (6)	0.0243 (6)	−0.0015 (5)	−0.0038 (5)	0.0050 (5)
N3	0.0246 (6)	0.0163 (6)	0.0217 (6)	−0.0005 (4)	−0.0008 (4)	0.0039 (5)
N4	0.0611 (11)	0.0437 (9)	0.0330 (8)	−0.0104 (8)	0.0139 (7)	−0.0058 (7)
O1	0.0453 (7)	0.0413 (7)	0.0234 (6)	0.0066 (6)	−0.0001 (5)	−0.0033 (5)
O2	0.0541 (7)	0.0304 (6)	0.0207 (5)	0.0052 (6)	−0.0027 (5)	0.0020 (5)
O3	0.0667 (11)	0.0791 (12)	0.0590 (10)	0.0140 (10)	0.0135 (8)	−0.0168 (9)
O4	0.1046 (13)	0.0585 (10)	0.0249 (7)	−0.0100 (9)	0.0117 (8)	−0.0095 (7)

Geometric parameters (Å, °)

C1—C2	1.376 (3)	C8—N2	1.3175 (19)
C1—C5	1.388 (2)	C8—N1	1.3414 (19)
C1—N4	1.463 (2)	C8—H8	0.9300
C2—C3	1.376 (3)	C9—N3	1.3149 (19)
C2—H2	0.9300	C9—N1	1.3478 (18)
C3—C4	1.386 (3)	C9—H9	0.9300
C3—H3	0.9300	Co1—O1	2.3314 (12)
C4—C6	1.385 (2)	Co1—O2	2.0008 (12)
C4—H4	0.9300	Co1—N1	2.0232 (12)
C5—C6	1.385 (2)	Co1—N2^{i}	2.0118 (12)
C5—H5	0.9300	Co1—N3^{ii}	2.0385 (12)
C6—C7	1.497 (2)	N2—N3	1.3759 (16)
C7—O1	1.243 (2)	N4—O3	1.212 (2)
C7—O2	1.272 (2)	N4—O4	1.229 (2)
C2—C1—C5	122.56 (17)	N1—C9—H9	123.7
C2—C1—N4	118.45 (17)	O2—Co1—N2^{i}	132.33 (5)
C5—C1—N4	118.98 (17)	O2—Co1—N1	109.04 (5)
C1—C2—C3	118.87 (17)	N2^{i}—Co1—N1	105.25 (5)
C1—C2—H2	120.6	O2—Co1—N3^{ii}	95.03 (5)
C3—C2—H2	120.6	N2^{i}—Co1—N3^{ii}	103.60 (5)
C2—C3—C4	119.79 (19)	N1—Co1—N3^{ii}	109.64 (5)
C2—C3—H3	120.1	O2—Co1—O1	60.06 (5)
C4—C3—H3	120.1	N2^{i}—Co1—O1	88.82 (5)
C6—C4—C3	120.72 (18)	N1—Co1—O1	89.18 (5)
C6—C4—H4	119.6	N3^{ii}—Co1—O1	153.26 (5)
C3—C4—H4	119.6	C8—N1—C9	102.90 (12)
C6—C5—C1	117.93 (16)	C8—N1—Co1	128.95 (10)
C6—C5—H5	121.0	C9—N1—Co1	127.60 (10)
C1—C5—H5	121.0	C8—N2—N3	106.17 (12)
C4—C6—C5	120.10 (15)	C8—N2—Co1^{iii}	124.78 (10)
C4—C6—C7	118.83 (15)	N3—N2—Co1^{iii}	128.36 (9)
C5—C6—C7	121.04 (15)	C9—N3—N2	105.91 (11)
O1—C7—O2	120.80 (14)	C9—N3—Co1^{iv}	125.40 (10)
O1—C7—C6	120.56 (15)	N2—N3—Co1^{iv}	128.05 (9)
O2—C7—C6	118.63 (15)	O3—N4—O4	123.81 (19)
N2—C8—N1	112.47 (13)	O3—N4—C1	118.64 (17)
N2—C8—H8	123.8	O4—N4—C1	117.55 (19)
N1—C8—H8	123.8	C7—O1—Co1	82.34 (10)
N3—C9—N1	112.56 (13)	C7—O2—Co1	96.61 (10)
N3—C9—H9	123.7		
C5—C1—C2—C3	−0.2 (3)	C7—Co1—N1—C9	25.56 (14)
N4—C1—C2—C3	178.90 (19)	N1—C8—N2—N3	0.24 (17)
C1—C2—C3—C4	−1.2 (3)	N1—C8—N2—Co1^{iii}	−170.88 (10)

C2—C3—C4—C6	1.7 (3)	N1—C9—N3—N2	−0.56 (17)
C2—C1—C5—C6	1.2 (3)	N1—C9—N3—Co1^{iv}	170.84 (10)
N4—C1—C5—C6	−177.94 (16)	C8—N2—N3—C9	0.19 (16)
C3—C4—C6—C5	−0.7 (3)	Co1^{iii}—N2—N3—C9	170.89 (10)
C3—C4—C6—C7	−178.94 (19)	C8—N2—N3—Co1^{iv}	−170.91 (10)
C1—C5—C6—C4	−0.7 (3)	Co1^{iii}—N2—N3—Co1^{iv}	−0.21 (18)
C1—C5—C6—C7	177.51 (16)	C2—C1—N4—O3	166.47 (19)
C4—C6—C7—O1	−10.4 (2)	C5—C1—N4—O3	−14.4 (3)
C5—C6—C7—O1	171.35 (16)	C2—C1—N4—O4	−14.4 (3)
C4—C6—C7—O2	168.80 (16)	C5—C1—N4—O4	164.78 (17)
C5—C6—C7—O2	−9.4 (2)	O2—C7—O1—Co1	−4.03 (15)
N2—C8—N1—C9	−0.55 (17)	C6—C7—O1—Co1	175.16 (15)
N2—C8—N1—Co1	171.29 (10)	O2—Co1—O1—C7	2.54 (10)
N3—C9—N1—C8	0.68 (17)	N2^{i}—Co1—O1—C7	−139.56 (10)
N3—C9—N1—Co1	−171.31 (10)	N1—Co1—O1—C7	115.17 (10)
O2—Co1—N1—C8	−113.76 (13)	N3^{ii}—Co1—O1—C7	−20.77 (16)
N2^{i}—Co1—N1—C8	99.90 (13)	O1—C7—O2—Co1	4.68 (18)
N3^{ii}—Co1—N1—C8	−10.96 (14)	C6—C7—O2—Co1	−174.52 (13)
O1—Co1—N1—C8	−171.55 (13)	N2^{i}—Co1—O2—C7	53.70 (13)
O2—Co1—N1—C9	56.19 (14)	N1—Co1—O2—C7	−79.98 (11)
N2^{i}—Co1—N1—C9	−90.15 (13)	N3^{ii}—Co1—O2—C7	167.23 (10)
N3^{ii}—Co1—N1—C9	158.99 (12)	O1—Co1—O2—C7	−2.47 (9)
O1—Co1—N1—C9	−1.60 (13)		

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1; (ii) −*x*+1/2, *y*−1/2, *z*; (iii) *x*+1/2, −*y*+3/2, −*z*+1; (iv) −*x*+1/2, *y*+1/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{v}	0.93	2.54	3.250 (3)	134
C8—H8···O4^{vi}	0.93	2.46	3.372 (2)	169

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

Fig. 1

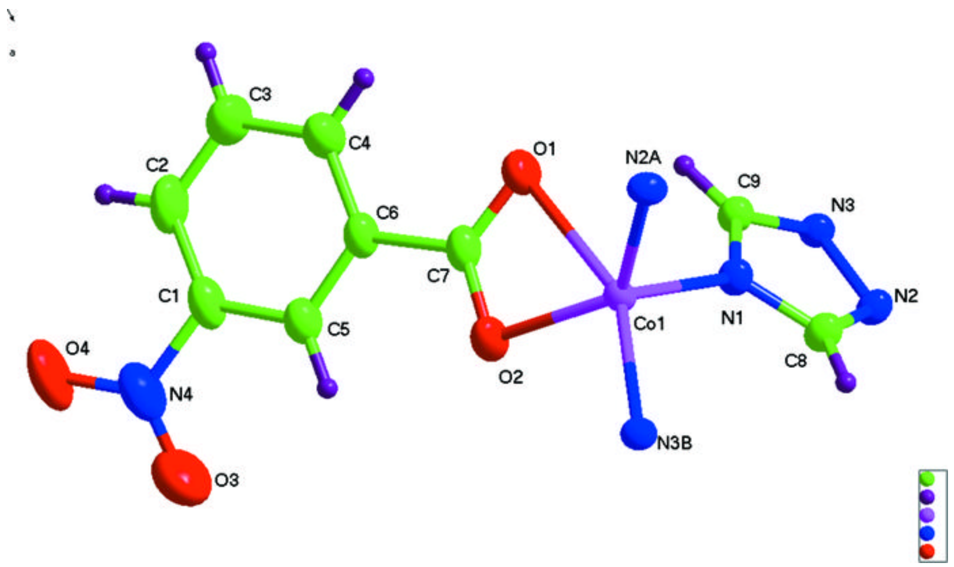

Fig. 2