Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[(3,5-dinitrobenzoato)-μ_3-triazolato-cobalt(II)]

Xu-Liang Qi

Liaocheng Vocational and Technical College, Liaocheng, Shandong, People's Republic of China
Correspondence e-mail: q200801@sina.com

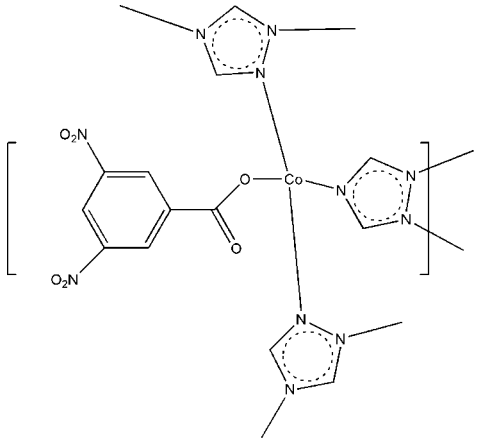
Received 30 November 2008; accepted 8 December 2008

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.026; wR factor = 0.060; data-to-parameter ratio = 13.7.

The title compound, $[Co(C_2H_2N_3)(C_7H_3N_2O_6)]_n$, was obtained by the reaction of $CoCl_2$, triazole and 3,5-dinitrobenzoic acid in a 1:1:1 ratio. The Co centre is in a distorted tetrahedral coordination by three N atoms of three different triazole ligands and one O atom of the 3,5-dinitrobenzoate anion.

Related literature

For background, see: Park *et al.* (2006).



Experimental

Crystal data

$[Co(C_2H_2N_3)(C_7H_3N_2O_6)]$
M_r = 338.11
Monoclinic, $P2_1/c$
a = 11.326 (2) Å
b = 9.4043 (19) Å
c = 10.696 (2) Å
β = 91.22 (3)°
V = 1139.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 296 (2) K
0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.812, T_{max} = 0.861
10929 measured reflections
2602 independent reflections
2256 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.060
S = 1.03
2602 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2826).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Park, H., Moureau, D. M. & Parise, J. B. (2006). *Chem. Mater.* **18**, 525–531.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2009). E**65**, m47 [**doi:10.1107/S160053680804155X**]

Poly[(3,5-dinitrobenzoato)-μ_3-triazolato-cobalt(II)]

X.-L. Qi

Comment

The asymmetric unit of the title compound is shown in Fig. 1. Co is four-coordinated by one O atom of a 3,5-dinitrobenzoic acid anion and three triazole N atoms in a tetrahedral geometry. The Co—O/N bond lengths of 1.9510 (13)–2.0396 (16)Å are in the normal range. The triazole and 3,5-dinitrobenzoic acid ligands adopt tridentate and monodentate coordinating modes, respectively. As shown in Figs. 2a and 2b, cobalt ions are connected by triazole ligands to generate a two-dimensional net with the 3,5-dinitrobenzoic acid ligands stacking out of this net. There is not obvious supramolecular interaction between the two-dimensional nets.

Experimental

$CoCl_2$ (1.0 mmol), 3,5-dinitrobenzoic acid (1 mmol), and triazole (1 mmol) were dissolved in water (10 ml). The solution was heated in a 25 ml Teflon lined reaction vessel at 433 K for *ca* 3 days and then cooled to room temperature. Purple crystals were obtained in a yield of 85%.

Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

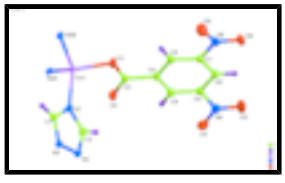


Fig. 1. An *ORTEP* view of the asymmetric unit with 50% displacement ellipsoids for non-H atoms. Symmetry codes: (A) -*x*,*y* - 1/2,-*z* + 1/2; (B) *x*,-*y* + 1/2,*z* + 1/2.

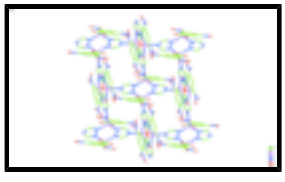


Fig. 2. View of the two-dimensional net.

Poly[(3,5-dinitrobenzoato)-μ$_3$-triazolato-cobalt(II)]

Crystal data

$[Co(C_2H_2N_3)(C_7H_3N_2O_6)]$ F_{000} = 676

M_r = 338.11	D_x = 1.972 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.326 (2) Å	Cell parameters from 8661 reflections
b = 9.4043 (19) Å	θ = 3.4–27.5º
c = 10.696 (2) Å	μ = 1.55 mm^{-1}
β = 91.22 (3)º	T = 296 (2) K
V = 1139.0 (4) Å^3	Block, red
Z = 4	0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2256 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 296(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.4º
Absorption correction: Multi-scan (SADABS; Sheldrick, 2004)	h = −14→14
T_{min} = 0.812, T_{max} = 0.861	k = −12→12
10929 measured reflections	l = −13→13
2602 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.026	H-atom parameters constrained
$wR(F^2)$ = 0.060	$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2 + 0.8847P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2602 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −0.36 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	−0.01347 (15)	0.35028 (19)	0.25548 (18)	0.0159 (4)
H1	−0.0595	0.3768	0.3226	0.019*
C2	0.10642 (16)	0.24145 (19)	0.14215 (18)	0.0176 (4)
H2	0.1617	0.1761	0.1145	0.021*
C3	0.32087 (15)	0.02322 (19)	0.30024 (19)	0.0187 (4)
C4	0.45442 (15)	0.03032 (19)	0.29392 (19)	0.0174 (4)
C5	0.51022 (16)	−0.0334 (2)	0.19406 (19)	0.0186 (4)

H5	0.4668	−0.0830	0.1335	0.022*
C6	0.52033 (16)	0.1050 (2)	0.38296 (19)	0.0181 (4)
H6	0.4838	0.1486	0.4499	0.022*
C7	0.64177 (16)	0.1134 (2)	0.37020 (19)	0.0185 (4)
C8	0.70035 (16)	0.0510 (2)	0.27338 (19)	0.0199 (4)
H8	0.7819	0.0574	0.2668	0.024*
C9	0.63179 (16)	−0.0217 (2)	0.18643 (19)	0.0195 (4)
Co1	0.10473 (2)	0.09672 (2)	0.39456 (2)	0.01158 (8)
N1	0.05927 (13)	0.23721 (15)	0.25698 (14)	0.0148 (3)
N2	0.06612 (12)	0.34762 (16)	0.07340 (14)	0.0142 (3)
N3	−0.01218 (12)	0.41947 (15)	0.14790 (14)	0.0140 (3)
N4	0.69050 (14)	−0.08206 (18)	0.07799 (17)	0.0236 (4)
N5	0.71165 (14)	0.19524 (18)	0.46234 (16)	0.0217 (4)
O1	0.27667 (11)	0.08348 (14)	0.39657 (14)	0.0209 (3)
O2	0.26354 (12)	−0.03470 (16)	0.21590 (14)	0.0270 (3)
O3	0.79840 (13)	−0.0720 (2)	0.07570 (16)	0.0399 (4)
O4	0.63013 (13)	−0.13889 (16)	−0.00391 (14)	0.0277 (3)
O5	0.65828 (13)	0.25969 (17)	0.54211 (16)	0.0339 (4)
O6	0.81961 (12)	0.19449 (16)	0.45430 (15)	0.0296 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0157 (8)	0.0187 (8)	0.0137 (9)	0.0024 (7)	0.0040 (7)	0.0001 (7)
C2	0.0198 (9)	0.0189 (9)	0.0144 (9)	0.0055 (7)	0.0045 (7)	0.0008 (7)
C3	0.0146 (8)	0.0190 (9)	0.0226 (10)	0.0003 (7)	0.0033 (7)	0.0074 (8)
C4	0.0144 (8)	0.0176 (8)	0.0202 (10)	0.0012 (7)	0.0023 (7)	0.0035 (8)
C5	0.0176 (8)	0.0192 (9)	0.0190 (10)	0.0008 (7)	0.0001 (7)	0.0011 (8)
C6	0.0161 (8)	0.0188 (9)	0.0194 (10)	0.0029 (7)	0.0027 (7)	0.0019 (8)
C7	0.0155 (8)	0.0205 (9)	0.0194 (10)	0.0001 (7)	−0.0015 (7)	0.0034 (8)
C8	0.0135 (8)	0.0246 (9)	0.0217 (10)	0.0032 (8)	0.0020 (7)	0.0050 (8)
C9	0.0188 (9)	0.0214 (9)	0.0184 (10)	0.0058 (8)	0.0044 (7)	0.0024 (8)
Co1	0.01125 (12)	0.01384 (12)	0.00973 (13)	−0.00079 (9)	0.00236 (8)	0.00031 (9)
N1	0.0168 (7)	0.0157 (7)	0.0120 (8)	0.0016 (6)	0.0038 (6)	0.0011 (6)
N2	0.0142 (7)	0.0166 (7)	0.0120 (8)	0.0020 (6)	0.0036 (6)	−0.0009 (6)
N3	0.0129 (7)	0.0174 (7)	0.0117 (8)	0.0025 (6)	0.0036 (6)	−0.0008 (6)
N4	0.0217 (8)	0.0280 (9)	0.0211 (9)	0.0074 (7)	0.0047 (7)	0.0026 (7)
N5	0.0196 (8)	0.0230 (8)	0.0225 (9)	−0.0005 (7)	−0.0021 (7)	0.0034 (7)
O1	0.0128 (6)	0.0242 (7)	0.0260 (8)	0.0001 (5)	0.0055 (5)	−0.0001 (6)
O2	0.0178 (6)	0.0368 (8)	0.0265 (8)	−0.0064 (6)	−0.0004 (6)	0.0003 (7)
O3	0.0182 (7)	0.0697 (12)	0.0321 (10)	0.0115 (8)	0.0057 (6)	−0.0112 (9)
O4	0.0324 (8)	0.0299 (7)	0.0210 (8)	0.0010 (6)	0.0032 (6)	−0.0035 (6)
O5	0.0308 (8)	0.0380 (9)	0.0329 (9)	0.0016 (7)	−0.0004 (7)	−0.0153 (7)
O6	0.0157 (6)	0.0387 (8)	0.0343 (9)	−0.0033 (6)	−0.0041 (6)	0.0045 (7)

Geometric parameters (Å, °)

C1—N3	1.322 (2)	C7—N5	1.469 (3)
C1—N1	1.345 (2)	C8—C9	1.380 (3)

C1—H1	0.9300	C8—H8	0.9300
C2—N2	1.316 (2)	C9—N4	1.464 (3)
C2—N1	1.350 (2)	Co1—O1	1.9510 (13)
C2—H2	0.9300	Co1—N3^{i}	2.0158 (15)
C3—O2	1.228 (2)	Co1—N1	2.0356 (16)
C3—O1	1.287 (2)	Co1—N2^{ii}	2.0396 (16)
C3—C4	1.517 (2)	N2—N3	1.381 (2)
C4—C6	1.388 (3)	N2—Co1^{iii}	2.0396 (16)
C4—C5	1.389 (3)	N3—Co1^{iv}	2.0158 (15)
C5—C9	1.385 (3)	N4—O4	1.223 (2)
C5—H5	0.9300	N4—O3	1.227 (2)
C6—C7	1.387 (3)	N5—O5	1.218 (2)
C6—H6	0.9300	N5—O6	1.228 (2)
C7—C8	1.373 (3)		
N3—C1—N1	112.41 (16)	C8—C9—N4	117.87 (16)
N3—C1—H1	123.8	C5—C9—N4	118.99 (18)
N1—C1—H1	123.8	O1—Co1—N3^{i}	117.64 (6)
N2—C2—N1	113.05 (16)	O1—Co1—N1	106.65 (6)
N2—C2—H2	123.5	N3^{i}—Co1—N1	104.57 (6)
N1—C2—H2	123.5	O1—Co1—N2^{ii}	103.88 (7)
O2—C3—O1	125.11 (17)	N3^{i}—Co1—N2^{ii}	107.62 (6)
O2—C3—C4	119.94 (18)	N1—Co1—N2^{ii}	117.09 (6)
O1—C3—C4	114.94 (17)	C1—N1—C2	102.70 (15)
C6—C4—C5	119.94 (17)	C1—N1—Co1	131.85 (13)
C6—C4—C3	120.92 (17)	C2—N1—Co1	125.30 (12)
C5—C4—C3	119.07 (17)	C2—N2—N3	105.55 (15)
C9—C5—C4	118.70 (18)	C2—N2—Co1^{iii}	129.80 (12)
C9—C5—H5	120.7	N3—N2—Co1^{iii}	124.66 (11)
C4—C5—H5	120.7	C1—N3—N2	106.29 (14)
C7—C6—C4	118.76 (18)	C1—N3—Co1^{iv}	125.99 (12)
C7—C6—H6	120.6	N2—N3—Co1^{iv}	127.71 (12)
C4—C6—H6	120.6	O4—N4—O3	124.17 (18)
C8—C7—C6	123.08 (18)	O4—N4—C9	118.73 (16)
C8—C7—N5	117.89 (17)	O3—N4—C9	117.10 (17)
C6—C7—N5	119.01 (18)	O5—N5—O6	124.19 (18)
C7—C8—C9	116.48 (17)	O5—N5—C7	117.56 (16)
C7—C8—H8	121.8	O6—N5—C7	118.25 (17)
C9—C8—H8	121.8	C3—O1—Co1	115.13 (12)
C8—C9—C5	123.05 (18)		
O2—C3—C4—C6	174.83 (18)	N3^{i}—Co1—N1—C2	−81.85 (15)
O1—C3—C4—C6	−3.9 (3)	N2^{ii}—Co1—N1—C2	159.19 (14)
O2—C3—C4—C5	−2.1 (3)	N1—C2—N2—N3	0.6 (2)
O1—C3—C4—C5	179.20 (17)	N1—C2—N2—Co1^{iii}	−179.28 (12)
C6—C4—C5—C9	0.6 (3)	N1—C1—N3—N2	0.1 (2)
C3—C4—C5—C9	177.53 (16)	N1—C1—N3—Co1^{iv}	−178.75 (11)

C5—C4—C6—C7	−0.4 (3)	C2—N2—N3—C1	−0.41 (18)
C3—C4—C6—C7	−177.31 (17)	Co1^{iii}—N2—N3—C1	179.45 (12)
C4—C6—C7—C8	−0.1 (3)	C2—N2—N3—Co1^{iv}	178.44 (12)
C4—C6—C7—N5	178.47 (17)	Co1^{iii}—N2—N3—Co1^{iv}	−1.7 (2)
C6—C7—C8—C9	0.4 (3)	C8—C9—N4—O4	−175.39 (17)
N5—C7—C8—C9	−178.19 (16)	C5—C9—N4—O4	1.3 (3)
C7—C8—C9—C5	−0.2 (3)	C8—C9—N4—O3	4.7 (3)
C7—C8—C9—N4	176.34 (17)	C5—C9—N4—O3	−178.66 (18)
C4—C5—C9—C8	−0.3 (3)	C8—C7—N5—O5	174.23 (18)
C4—C5—C9—N4	−176.77 (17)	C6—C7—N5—O5	−4.4 (3)
N3—C1—N1—C2	0.2 (2)	C8—C7—N5—O6	−5.8 (3)
N3—C1—N1—Co1	175.77 (12)	C6—C7—N5—O6	175.59 (17)
N2—C2—N1—C1	−0.5 (2)	O2—C3—O1—Co1	−6.3 (2)
N2—C2—N1—Co1	−176.45 (12)	C4—C3—O1—Co1	172.33 (11)
O1—Co1—N1—C1	−131.24 (16)	N3^{i}—Co1—O1—C3	48.42 (14)
N3^{i}—Co1—N1—C1	103.46 (16)	N1—Co1—O1—C3	−68.51 (13)
N2^{ii}—Co1—N1—C1	−15.50 (18)	N2^{ii}—Co1—O1—C3	167.19 (12)
O1—Co1—N1—C2	43.46 (16)		

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

Fig. 1

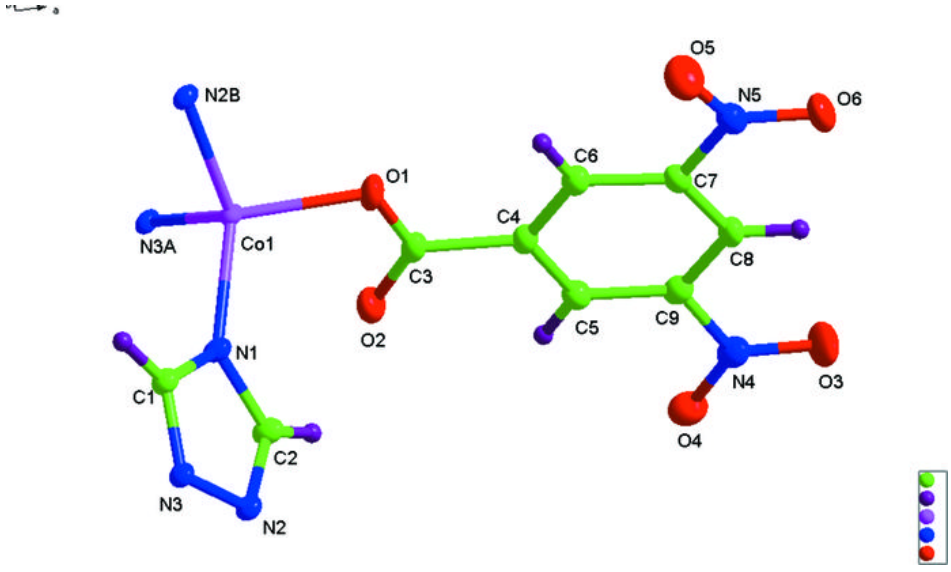
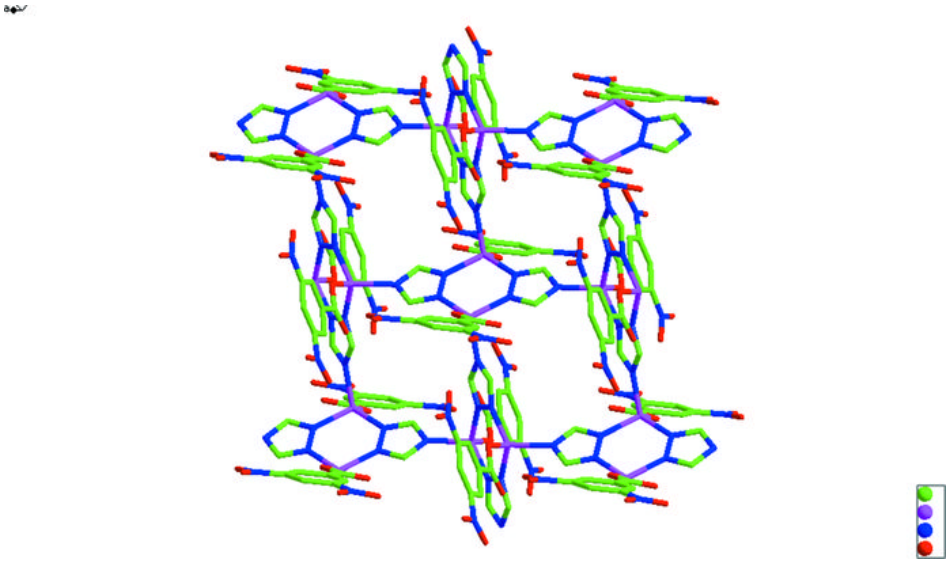



Fig. 2