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

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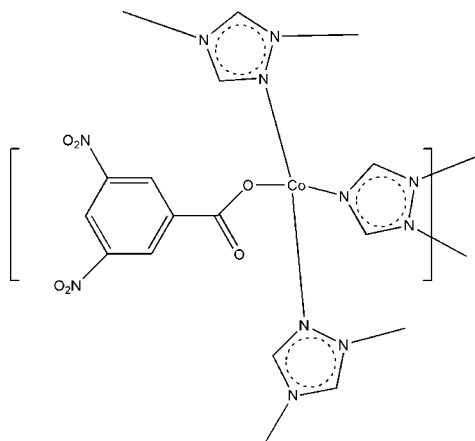
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.026; wR factor = 0.060; data-to-parameter ratio = 13.7.

The title compound, $[\text{Co}(\text{C}_2\text{H}_2\text{N}_3)(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)]_n$, 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

 $[\text{Co}(\text{C}_2\text{H}_2\text{N}_3)(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)]$
 $M_r = 338.11$

 Monoclinic, $P2_1/c$
 $a = 11.326$ (2) Å

 $b = 9.4043$ (19) Å

 $c = 10.696$ (2) Å

 $\beta = 91.22$ (3)°

 $V = 1139.0$ (4) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 1.55$ mm⁻¹
 $T = 296$ (2) K

 $0.14 \times 0.12 \times 0.10$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$

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

 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.36$ 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.* **A64**, 112–122.

supporting information

Acta Cryst. (2009). E65, m47 [doi:10.1107/S160053680804155X]

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

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S1. 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.

S2. Experimental

CoCl₂ (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%.

S3. Refinement

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

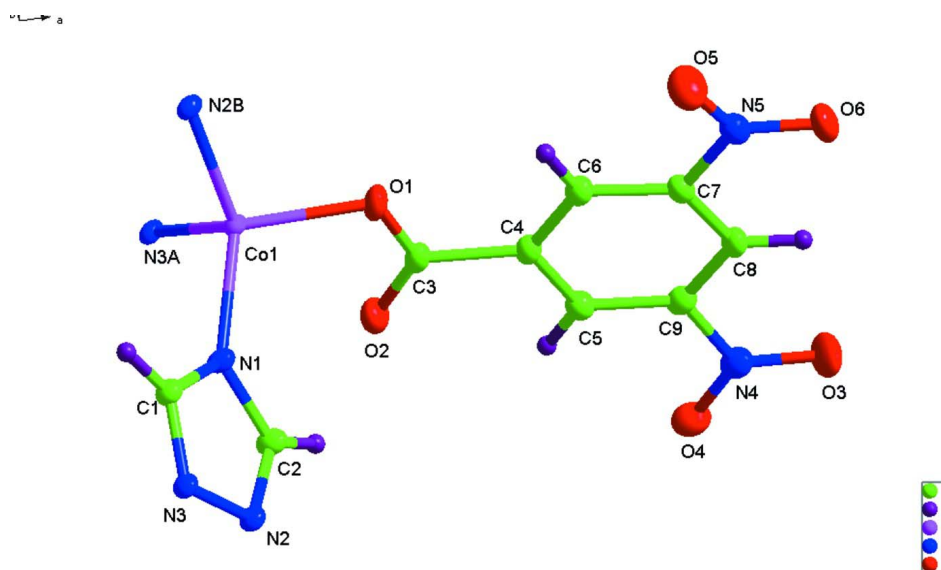
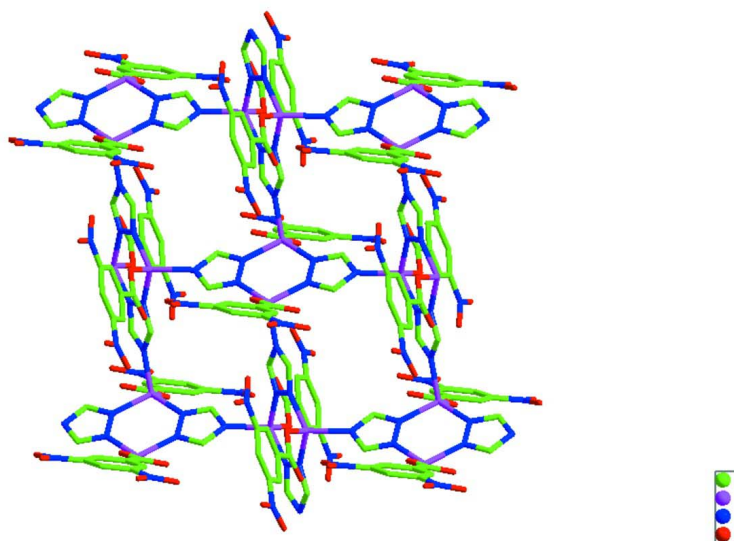


Figure 1

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) $x, -y + 1/2, z + 1/2$.

**Figure 2**

View of the two-dimensional net.

Poly[(3,5-dinitrobenzoato)- μ_3 -triazolato-cobalt(II)]*Crystal data*[Co(C₂H₂N₃)(C₇H₃N₂O₆)] $M_r = 338.11$ Monoclinic, $P2_1/c$ $a = 11.326 (2) \text{ \AA}$ $b = 9.4043 (19) \text{ \AA}$ $c = 10.696 (2) \text{ \AA}$ $\beta = 91.22 (3)^\circ$ $V = 1139.0 (4) \text{ \AA}^3$ $Z = 4$ $F(000) = 676$ $D_x = 1.972 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 8661 reflections

 $\theta = 3.4\text{--}27.5^\circ$ $\mu = 1.55 \text{ mm}^{-1}$ $T = 296 \text{ K}$

Block, red

 $0.14 \times 0.12 \times 0.10 \text{ mm}$ *Data collection*Bruker SMART 1K CCD area-detector
diffractometer

Radiation source: rotating anode

Graphite monochromator

 ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 2004)

 $T_{\min} = 0.812$, $T_{\max} = 0.861$

10929 measured reflections

2602 independent reflections

2256 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.041$ $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.4^\circ$ $h = -14 \rightarrow 14$ $k = -12 \rightarrow 12$ $l = -13 \rightarrow 13$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.026$ $wR(F^2) = 0.060$ $S = 1.03$

2602 reflections

190 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2 + 0.8847P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.33 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^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) $-x, y+1/2, -z+1/2$.