

Poly[bis[μ_2 -1,4-bis(1,2,4-triazol-1-yl-methyl)benzene- $\kappa^2N^4:N^4'$]bis(nitrito- κO)cobalt(II)]

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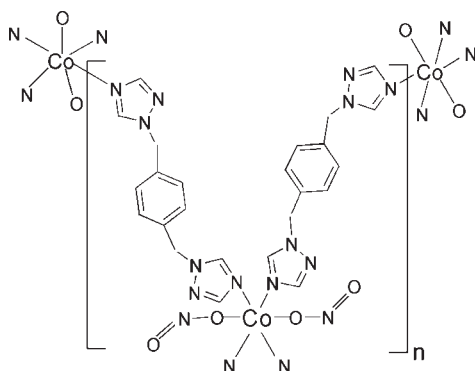
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Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(C-C) = 0.003$ Å; R factor = 0.041; wR factor = 0.098; data-to-parameter ratio = 16.0.

The Co^{II} atom in the title complex, $[Co(NO_2)_2(C_{12}H_{12}N_6)_2]_n$, lies on an inversion center and is coordinated by four N atoms from the triazole rings of two symmetry-related pairs of 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) ligands and two O atoms from two symmetry-related monodentate nitrate ligands in a distorted octahedral geometry. The Co atoms are bridged by four bbtz ligands, forming a two-dimensional (4,4) network parallel to (102).

Related literature

The synthesis of the ligand 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) was described by Peng *et al.* (2004). Several bbtz complexes have been synthesized and structurally characterized, see: Li *et al.* (2005); Wang *et al.* (2007).



Experimental

Crystal data

$[Co(NO_2)_2(C_{12}H_{12}N_6)_2]$
 $M_r = 631.50$
 Monoclinic, $P2_1/c$
 $a = 8.3037$ (13) Å
 $b = 20.376$ (3) Å
 $c = 8.4261$ (11) Å
 $\beta = 104.390$ (4)°

$V = 1380.9$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.68$ mm⁻¹
 $T = 193$ K
 $0.33 \times 0.26 \times 0.10$ mm

Data collection

Rigaku Mercury CCD diffractometer
 Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
 $T_{min} = 0.806$, $T_{max} = 0.935$

15379 measured reflections
 3152 independent reflections
 2768 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.098$
 $S = 1.07$
 3152 reflections

197 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.28$ e Å⁻³
 $\Delta\rho_{min} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.1031 (15)	Co1—N3	2.1530 (16)
Co1—N6 ⁱ	2.1418 (16)		
O1 ⁱⁱ —Co1—O1	180	O1—Co1—N3	93.70 (6)
O1—Co1—N6 ⁱ	85.99 (6)	N6 ⁱ —Co1—N3	90.52 (6)
N6 ⁱ —Co1—N6 ⁱⁱⁱ	180	N3—Co1—N3 ⁱⁱ	180

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

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2227).

References

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supplementary materials

Acta Cryst. (2010). E66, m85 [doi:10.1107/S1600536809039415]

Poly[bis[μ_2 -1,4-bis(1,2,4-triazol-1-ylmethyl)benzene- $\kappa^2N^4:N^4'$]bis(nitrito- κO)cobalt(II)]

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Comment

The title compound is isostructural with its azido Ni^{II} analog (Wang *et al.*, 2007).

Fig. 1 shows the local coordination of the Co^{II} atom. In the complex the Co^{II} atom occupies an inversion center. The coordination geometry of the Co^{II} atom is a distorted octahedron. Each Co^{II} atom is coordinated equatorial by four nitrogen atoms from the triazole rings of four bbtz ligands [Co1—N3, 2.1530 (16) Å; Co1—N6 (-x + 1, y - 1/2, -z + 1/2), 2.1418 (16) Å], and axially by two oxygen atoms from two symmetry-related nitrite anions [Co1—O1, 2.1031 (15) Å]. The bbtz ligands shows the *trans-gauche* conformation, similar to the uncoordinated bbtz molecule (Peng *et al.*, 2004).

As illustrated in Fig.2, each bbtz ligand coordinated to the Co^{II} atoms through its two triazole nitrogen atoms, thus acting as a bridging bidentate ligand to form a two-dimensional (4,4) network. As a consequence of the symmetry of the crystal structure, the edge lengths are equal, with a value of 14.4182 (14) Å. The square-grid sheets are stacked in an offset fashion parallel to the c direction. The off-set half-cell superposition of each pair of adjacent networks divides the voids into smaller rectangle. The nitrile anions of one sheet project into the holes of the next sheet. In the superposition structure, the sheets are arranged in the sequence "A—B—A—B" (Fig.3).

Experimental

A H₂O/MeOH solution (20 ml, 1:1 v/v) of Co(ClO₄)₂·6H₂O (0.50 mmol) and NaNO₂ (2.0 mmol) was added to one leg of a "H-shaped" tube, and a H₂O/MeOH solution (20 ml, 1:1 v/v) of bbtz (0.240 g, 1.00 mmol) was added to the other leg of the tube. After several weeks, the well shaped red single crystals were obtained. Found: C, 45.57; H, 3.79; N, 30.94%. Calcd. for C₂₄H₂₄C₆N₁₄O₄: C, 45.65; H, 3.83; N, 31.06%.

Refinement

H atoms were placed in idealized positions and refined as riding, with C—H distances of 0.95 (triazole and benzene) and 0.99 Å (methyl), and with $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C})$.

Figures

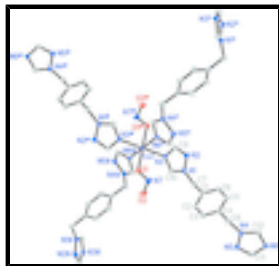


Fig. 1. The coordination environment of the Co^{II} atom in the title compound. Ellipsoids are drawn at the 30% probability level. [Symmetry codes # $-x, -y + 1, -z + 1$; \$ $-x + 1, y - 1/2, -z + 1/2$; * $x - 1, -y + 3/2, z + 1/2$]. The hydrogen atoms have been omitted for clarity.

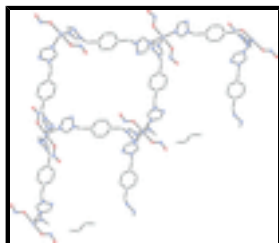


Fig. 2. View of the two-dimensional (4,4) network of the title compound along the c direction.

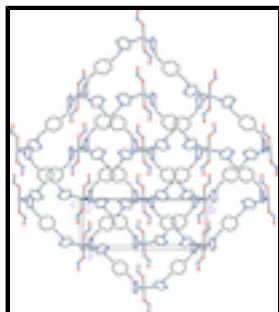


Fig. 3. The cell packing of the title compound.

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$b = 20.376$ (3) Å

$c = 8.4261$ (11) Å

$\beta = 104.390$ (4)°

$V = 1380.9$ (3) Å³

$Z = 2$

$F(000) = 650$

$D_x = 1.519$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5616 reflections

$\theta = 3.1$ – 27.5 °

$\mu = 0.68$ mm⁻¹

$T = 193$ K

Block, red

$0.33 \times 0.26 \times 0.10$ mm

Data collection

Rigaku Mercury CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

3152 independent reflections

2768 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

ω scans	$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.2^\circ$
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	$h = -10 \rightarrow 10$
$T_{\min} = 0.806$, $T_{\max} = 0.935$	$k = -26 \rightarrow 26$
15379 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.098$	H-atom parameters constrained
$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.7485P]$
3152 reflections	where $P = (F_o^2 + 2F_c^2)/3$
197 parameters	$(\Delta/\sigma)_{\max} < 0.001$
0 restraints	$\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.0000	0.5000	0.5000	0.02085 (12)
O1	0.25015 (18)	0.50405 (7)	0.6333 (2)	0.0350 (4)
O2	0.48900 (19)	0.54314 (9)	0.7278 (2)	0.0461 (4)
N1	0.1620 (2)	0.57944 (8)	0.0939 (2)	0.0273 (4)
N2	-0.0036 (2)	0.58502 (11)	0.0290 (2)	0.0412 (5)
N3	0.0484 (2)	0.54604 (8)	0.2865 (2)	0.0257 (3)
N4	0.8222 (2)	0.83452 (8)	0.2102 (2)	0.0274 (4)
N5	0.9542 (2)	0.80233 (9)	0.1784 (2)	0.0349 (4)
N6	0.93982 (19)	0.90596 (8)	0.08323 (19)	0.0253 (3)
N7	0.3509 (2)	0.54893 (10)	0.6299 (2)	0.0425 (5)
C1	0.3965 (2)	0.65065 (10)	0.0737 (2)	0.0282 (4)
C2	0.5418 (3)	0.63661 (11)	0.1894 (3)	0.0343 (5)
H2A	0.5699	0.5923	0.2188	0.041*

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C3	0.6470 (3)	0.68667 (11)	0.2632 (3)	0.0339 (5)
H3A	0.7471	0.6762	0.3419	0.041*
C4	0.6084 (3)	0.75136 (10)	0.2239 (2)	0.0289 (4)
C5	0.4628 (3)	0.76574 (11)	0.1061 (3)	0.0376 (5)
H5A	0.4353	0.8101	0.0766	0.045*
C6	0.3576 (3)	0.71570 (11)	0.0315 (3)	0.0364 (5)
H6A	0.2585	0.7260	-0.0488	0.044*
C7	0.2823 (3)	0.59545 (11)	-0.0029 (3)	0.0333 (5)
H7A	0.2214	0.6082	-0.1151	0.040*
H7B	0.3494	0.5560	-0.0112	0.040*
C8	0.7201 (3)	0.80549 (11)	0.3108 (3)	0.0370 (5)
H8A	0.6508	0.8403	0.3425	0.044*
H8B	0.7939	0.7877	0.4125	0.044*
C9	-0.0655 (3)	0.56403 (12)	0.1496 (3)	0.0371 (5)
H9A	-0.1817	0.5618	0.1406	0.044*
C10	0.1907 (3)	0.55662 (11)	0.2456 (2)	0.0312 (5)
H10A	0.2979	0.5489	0.3153	0.037*
C11	1.0198 (3)	0.84752 (10)	0.1016 (3)	0.0317 (5)
H11A	1.1157	0.8397	0.0621	0.038*
C12	0.8157 (2)	0.89541 (10)	0.1543 (2)	0.0269 (4)
H12A	0.7344	0.9270	0.1635	0.032*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01814 (19)	0.02220 (19)	0.0236 (2)	-0.00012 (13)	0.00787 (14)	0.00201 (14)
O1	0.0210 (7)	0.0348 (8)	0.0459 (9)	-0.0049 (6)	0.0020 (6)	0.0075 (7)
O2	0.0229 (8)	0.0624 (11)	0.0527 (10)	-0.0088 (7)	0.0087 (7)	-0.0060 (9)
N1	0.0262 (9)	0.0307 (9)	0.0257 (8)	-0.0063 (7)	0.0079 (7)	0.0017 (7)
N2	0.0296 (10)	0.0549 (13)	0.0378 (10)	-0.0010 (9)	0.0058 (8)	0.0142 (9)
N3	0.0251 (8)	0.0266 (8)	0.0273 (8)	0.0002 (6)	0.0101 (6)	0.0036 (7)
N4	0.0262 (8)	0.0276 (8)	0.0291 (9)	-0.0053 (7)	0.0083 (7)	-0.0024 (7)
N5	0.0296 (9)	0.0304 (9)	0.0455 (11)	0.0004 (7)	0.0108 (8)	0.0020 (8)
N6	0.0221 (8)	0.0260 (8)	0.0289 (8)	-0.0026 (6)	0.0084 (6)	-0.0019 (7)
N7	0.0331 (10)	0.0523 (12)	0.0406 (11)	-0.0124 (9)	0.0061 (8)	0.0041 (9)
C1	0.0274 (10)	0.0323 (11)	0.0283 (10)	-0.0054 (8)	0.0135 (8)	0.0017 (8)
C2	0.0330 (11)	0.0293 (11)	0.0412 (12)	-0.0004 (9)	0.0101 (9)	0.0087 (9)
C3	0.0288 (11)	0.0365 (11)	0.0342 (11)	-0.0014 (9)	0.0034 (9)	0.0089 (9)
C4	0.0293 (10)	0.0314 (10)	0.0284 (10)	-0.0053 (8)	0.0118 (8)	0.0013 (8)
C5	0.0344 (12)	0.0282 (11)	0.0499 (14)	-0.0001 (9)	0.0098 (10)	0.0077 (10)
C6	0.0284 (11)	0.0389 (12)	0.0394 (12)	0.0001 (9)	0.0035 (9)	0.0091 (10)
C7	0.0368 (12)	0.0396 (12)	0.0281 (10)	-0.0116 (9)	0.0167 (9)	-0.0018 (9)
C8	0.0424 (13)	0.0397 (12)	0.0323 (11)	-0.0137 (10)	0.0154 (10)	-0.0017 (10)
C9	0.0244 (11)	0.0480 (13)	0.0404 (12)	0.0020 (9)	0.0110 (9)	0.0111 (10)
C10	0.0249 (10)	0.0411 (12)	0.0280 (10)	-0.0036 (8)	0.0069 (8)	0.0064 (9)
C11	0.0244 (10)	0.0303 (10)	0.0414 (12)	-0.0003 (8)	0.0099 (9)	-0.0019 (9)
C12	0.0242 (10)	0.0267 (10)	0.0309 (10)	-0.0022 (8)	0.0088 (8)	-0.0022 (8)

Geometric parameters (Å, °)

Co1—O1 ⁱ	2.1031 (15)	C1—C2	1.380 (3)
Co1—O1	2.1031 (15)	C1—C6	1.389 (3)
Co1—N6 ⁱⁱ	2.1418 (16)	C1—C7	1.509 (3)
Co1—N6 ⁱⁱⁱ	2.1418 (16)	C2—C3	1.385 (3)
Co1—N3	2.1530 (16)	C2—H2A	0.9500
Co1—N3 ⁱ	2.1530 (16)	C3—C4	1.377 (3)
O1—N7	1.245 (2)	C3—H3A	0.9500
O2—N7	1.240 (2)	C4—C5	1.391 (3)
N1—C10	1.325 (3)	C4—C8	1.509 (3)
N1—N2	1.353 (2)	C5—C6	1.387 (3)
N1—C7	1.475 (2)	C5—H5A	0.9500
N2—C9	1.319 (3)	C6—H6A	0.9500
N3—C10	1.328 (2)	C7—H7A	0.9900
N3—C9	1.348 (3)	C7—H7B	0.9900
N4—C12	1.324 (3)	C8—H8A	0.9900
N4—N5	1.360 (2)	C8—H8B	0.9900
N4—C8	1.465 (3)	C9—H9A	0.9500
N5—C11	1.319 (3)	C10—H10A	0.9500
N6—C12	1.331 (2)	C11—H11A	0.9500
N6—C11	1.353 (3)	C12—H12A	0.9500
N6—Co1 ^{iv}	2.1418 (16)		
O1 ⁱ —Co1—O1	180.0	C4—C3—C2	120.9 (2)
O1 ⁱ —Co1—N6 ⁱⁱ	94.01 (6)	C4—C3—H3A	119.6
O1—Co1—N6 ⁱⁱ	85.99 (6)	C2—C3—H3A	119.6
O1 ⁱ —Co1—N6 ⁱⁱⁱ	85.99 (6)	C3—C4—C5	118.83 (19)
O1—Co1—N6 ⁱⁱⁱ	94.01 (6)	C3—C4—C8	120.3 (2)
N6 ⁱⁱ —Co1—N6 ⁱⁱⁱ	180.00 (8)	C5—C4—C8	120.85 (19)
O1 ⁱ —Co1—N3	86.30 (6)	C6—C5—C4	120.4 (2)
O1—Co1—N3	93.70 (6)	C6—C5—H5A	119.8
N6 ⁱⁱ —Co1—N3	90.52 (6)	C4—C5—H5A	119.8
N6 ⁱⁱⁱ —Co1—N3	89.48 (6)	C5—C6—C1	120.3 (2)
O1 ⁱ —Co1—N3 ⁱ	93.70 (6)	C5—C6—H6A	119.8
O1—Co1—N3 ⁱ	86.30 (6)	C1—C6—H6A	119.8
N6 ⁱⁱ —Co1—N3 ⁱ	89.48 (6)	N1—C7—C1	111.64 (17)
N6 ⁱⁱⁱ —Co1—N3 ⁱ	90.52 (6)	N1—C7—H7A	109.3
N3—Co1—N3 ⁱ	180.00 (8)	C1—C7—H7A	109.3
N7—O1—Co1	126.67 (14)	N1—C7—H7B	109.3
C10—N1—N2	109.92 (16)	C1—C7—H7B	109.3
C10—N1—C7	128.82 (18)	H7A—C7—H7B	108.0
N2—N1—C7	121.23 (17)	N4—C8—C4	112.87 (17)
C9—N2—N1	102.28 (17)	N4—C8—H8A	109.0
C10—N3—C9	102.35 (17)	C4—C8—H8A	109.0

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C10—N3—Co1	130.55 (14)	N4—C8—H8B	109.0
C9—N3—Co1	126.63 (14)	C4—C8—H8B	109.0
C12—N4—N5	110.21 (16)	H8A—C8—H8B	107.8
C12—N4—C8	127.34 (18)	N2—C9—N3	115.02 (19)
N5—N4—C8	122.01 (17)	N2—C9—H9A	122.5
C11—N5—N4	102.19 (17)	N3—C9—H9A	122.5
C12—N6—C11	102.66 (16)	N3—C10—N1	110.43 (18)
C12—N6—Co1 ^{iv}	124.14 (13)	N3—C10—H10A	124.8
C11—N6—Co1 ^{iv}	132.60 (13)	N1—C10—H10A	124.8
O2—N7—O1	115.52 (19)	N5—C11—N6	114.82 (18)
C2—C1—C6	119.04 (19)	N5—C11—H11A	122.6
C2—C1—C7	119.60 (19)	N6—C11—H11A	122.6
C6—C1—C7	121.36 (19)	N4—C12—N6	110.11 (17)
C1—C2—C3	120.5 (2)	N4—C12—H12A	124.9
C1—C2—H2A	119.7	N6—C12—H12A	124.9
C3—C2—H2A	119.7		
N6 ⁱⁱ —Co1—O1—N7	126.75 (19)	C2—C1—C6—C5	-0.6 (3)
N6 ⁱⁱⁱ —Co1—O1—N7	-53.25 (19)	C7—C1—C6—C5	178.6 (2)
N3—Co1—O1—N7	36.48 (19)	C10—N1—C7—C1	-63.3 (3)
N3 ⁱ —Co1—O1—N7	-143.52 (19)	N2—N1—C7—C1	119.1 (2)
C10—N1—N2—C9	-0.5 (2)	C2—C1—C7—N1	88.2 (2)
C7—N1—N2—C9	177.54 (19)	C6—C1—C7—N1	-91.0 (2)
O1 ⁱ —Co1—N3—C10	-165.51 (19)	C12—N4—C8—C4	115.1 (2)
O1—Co1—N3—C10	14.49 (19)	N5—N4—C8—C4	-73.2 (3)
N6 ⁱⁱ —Co1—N3—C10	-71.53 (19)	C3—C4—C8—N4	104.3 (2)
N6 ⁱⁱⁱ —Co1—N3—C10	108.47 (19)	C5—C4—C8—N4	-77.4 (3)
O1 ⁱ —Co1—N3—C9	5.24 (18)	N1—N2—C9—N3	0.5 (3)
O1—Co1—N3—C9	-174.76 (18)	C10—N3—C9—N2	-0.3 (3)
N6 ⁱⁱ —Co1—N3—C9	99.22 (18)	Co1—N3—C9—N2	-173.14 (16)
N6 ⁱⁱⁱ —Co1—N3—C9	-80.78 (18)	C9—N3—C10—N1	0.0 (2)
C12—N4—N5—C11	-0.5 (2)	Co1—N3—C10—N1	172.41 (13)
C8—N4—N5—C11	-173.46 (18)	N2—N1—C10—N3	0.3 (3)
Co1—O1—N7—O2	175.00 (14)	C7—N1—C10—N3	-177.51 (18)
C6—C1—C2—C3	0.3 (3)	N4—N5—C11—N6	0.4 (2)
C7—C1—C2—C3	-178.94 (19)	C12—N6—C11—N5	-0.1 (2)
C1—C2—C3—C4	0.6 (3)	Co1 ^{iv} —N6—C11—N5	170.93 (14)
C2—C3—C4—C5	-1.2 (3)	N5—N4—C12—N6	0.5 (2)
C2—C3—C4—C8	177.2 (2)	C8—N4—C12—N6	172.95 (18)
C3—C4—C5—C6	0.9 (3)	C11—N6—C12—N4	-0.2 (2)
C8—C4—C5—C6	-177.4 (2)	Co1 ^{iv} —N6—C12—N4	-172.27 (12)
C4—C5—C6—C1	0.0 (3)		

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

Fig. 1

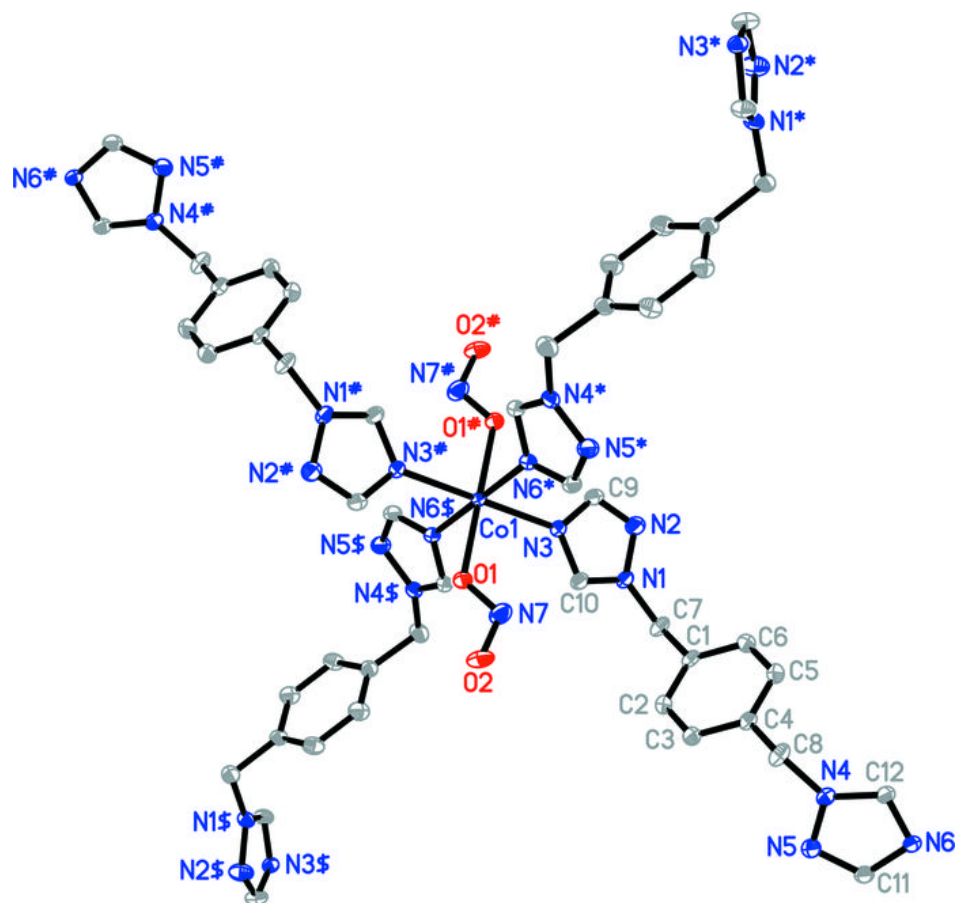


Fig. 2

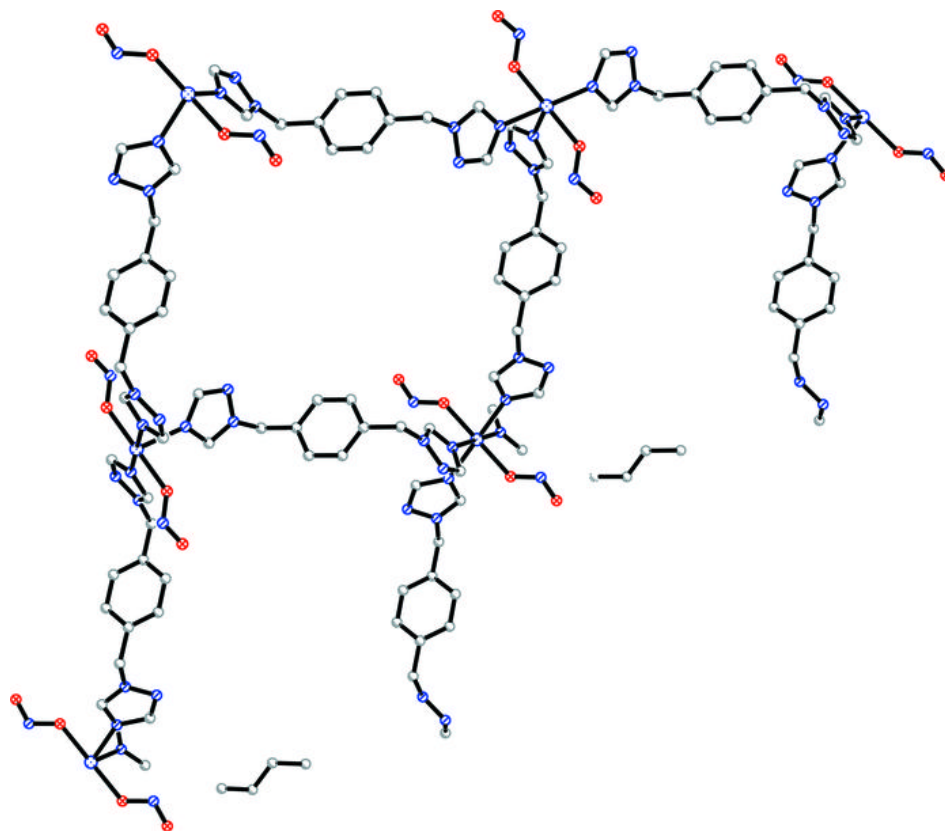


Fig. 3

