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Poly[[μ_2-1,2-bis(imidazol-1-ylmethyl)-benzene](μ_2-cyclohexane-1,4-dicarboxylato)cobalt(II)]

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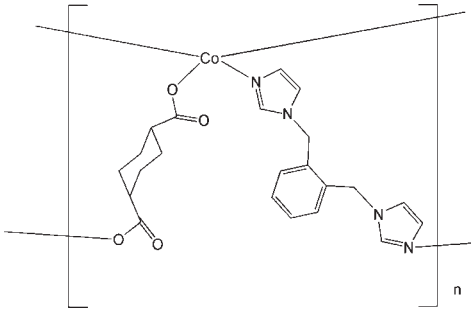
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 17.6.

In the the title compound, $[Co(C_8H_{10}O_4)(C_{14}H_{14}N_4)]_n$, the Co^{II} atom is four-coordinated by two N atoms from two different 1,2-bis(imidazol-1-ylmethyl)benzene ligands and two carboxylate O atoms from two different cyclohexane-1,4-dicarboxylate anions in a tetrahedral coordination geometry. The resulting structure is a two-dimensional polymer with layers in the (100) plane.

Related literature

For a related structure, see: Li *et al.* (2009).



Experimental

Crystal data

$[Co(C_8H_{10}O_4)(C_{14}H_{14}N_4)]$
M_r = 467.38
Monoclinic, $P2_1/c$
a = 9.785 (3) Å
b = 12.356 (2) Å
c = 17.850 (4) Å
β = 99.559 (2)°
V = 2128.2 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 293 K
0.27 × 0.21 × 0.17 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.51, T_{max} = 0.83
9866 measured reflections
4923 independent reflections
3485 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 0.96
4923 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; 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*.

We thank Jiangsu University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5196).

References

Li, B.-B., Fang, G.-X., Ji, X.-N., Xiao, B. & Tiekink, E. R. T. (2009). *Acta Cryst.* E**65**, m1012.
Oxford Diffraction (2006). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2010). E**66**, m330 [doi:10.1107/S160053681000646X]

Poly[[μ_2-1,2-bis(imidazol-1-ylmethyl)benzene](μ_2-cyclohexane-1,4-dicarboxylato)cobalt(II)]

Min Chen and Min Xing

S1. Comment

The flexible N-donor ligand, 1,2-bis(imidazol-1-ylmethyl)benzene is a good candidate for the construction of coordination polymers (Li *et al.*, 2009). We report here the synthesis and structure of the title compound, composed of this ligand, cyclohexane-1,4-dicarboxylate and Co atoms.

The Co^{II} atom is four-coordinated by two nitrogen atoms from two different 1,2-bis(imidazol-1-ylmethyl)benzene ligands and two carboxylate oxygen atoms from two different cyclohexane-1,4-dicarboxylate anions in a tetrahedral coordination geometry. The resulting structure is a two-dimensional polymer with layers in the (1 0 0) plane.

S2. Experimental

1,4-H_2chdc (0.5 mmol), 1,2-bix (0.5 mmol) and cobalt chloride hexahydrate (0.5 mmol) were placed in water (12 ml), and triethylamine was added until the pH value of the solution was 5.4. The solution was heated in a 23 ml Teflon-lined stainless-steel autoclave at 430 K for 5 days. The autoclave was cooled to room temperature over several hours. Purple crystals were isolated in about 38% yield.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93 to 0.98 Å) and refined as riding, with $U_{iso}(H)=1.2U_{eq}(C)$.

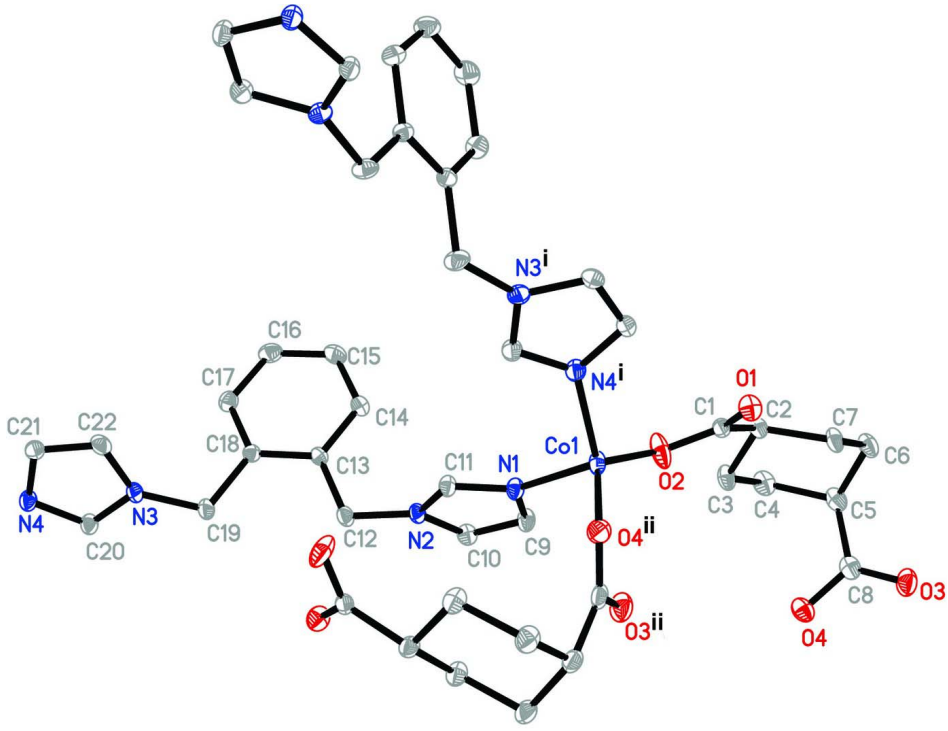


Figure 1

The structure of the title compound, showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i) x, -0.5-y, z-0.5; (ii) 1-x, y-0.5, 0.5-z.

Poly[[μ_2-1,2-bis(imidazol-1-ylmethyl)benzene](μ_2-cyclohexane-1,4- dicarboxylato)cobalt(II)]

Crystal data

$[Co(C_8H_{10}O_4)(C_{14}H_{14}N_4)]$
$M_r = 467.38$
Monoclinic, $P2_1/c$
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$b = 12.356$ (2) Å
$c = 17.850$ (4) Å
$\beta = 99.559$ (2)°
$V = 2128.2$ (9) Å^3
$Z = 4$
$F(000) = 972$
$D_x = 1.459$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4923 reflections
$\theta = 2.3$–$29.1°$
$\mu = 0.84$ mm^{-1}
$T = 293$ K
Block, purple
0.27 × 0.21 × 0.17 mm

Data collection

Oxford Diffraction Gemini R Ultra diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min} = 0.51$, $T_{max} = 0.83$
9866 measured reflections
4923 independent reflections
3485 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 29.1°$, $\theta_{min} = 2.3°$
$h = -8 \rightarrow 12$
$k = -16 \rightarrow 15$
$l = -23 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.079$
$S = 0.96$
4923 reflections
280 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.73125 (18)	0.35656 (12)	0.18015 (9)	0.0353 (4)
C2	0.82011 (19)	0.44982 (12)	0.21681 (8)	0.0372 (4)
H2	0.9170	0.4315	0.2151	0.045*
C3	0.8064 (2)	0.46346 (14)	0.30090 (9)	0.0452 (4)
H3A	0.7090	0.4687	0.3049	0.054*
H3B	0.8434	0.3996	0.3287	0.054*
C4	0.8814 (2)	0.56275 (15)	0.33757 (10)	0.0515 (5)
H4A	0.9805	0.5529	0.3407	0.062*
H4B	0.8621	0.5705	0.3889	0.062*
C5	0.8367 (2)	0.66551 (14)	0.29255 (10)	0.0476 (5)
H5	0.8949	0.7248	0.3162	0.057*
C6	0.8670 (2)	0.65185 (14)	0.21139 (10)	0.0513 (5)
H6A	0.8402	0.7171	0.1824	0.062*
H6B	0.9657	0.6411	0.2130	0.062*
C7	0.7878 (2)	0.55525 (13)	0.17234 (9)	0.0450 (5)
H7A	0.8115	0.5467	0.1220	0.054*
H7B	0.6892	0.5696	0.1665	0.054*
C8	0.6860 (2)	0.69815 (14)	0.29141 (10)	0.0460 (5)
C9	0.64364 (19)	0.15946 (12)	0.36882 (9)	0.0393 (4)
H9	0.6565	0.2340	0.3690	0.047*
C10	0.65119 (17)	0.09703 (13)	0.43108 (8)	0.0368 (4)
H10	0.6699	0.1200	0.4814	0.044*
C11	0.60365 (17)	−0.00366 (12)	0.32978 (8)	0.0340 (4)
H11	0.5836	−0.0639	0.2986	0.041*
C12	0.62805 (17)	−0.10377 (13)	0.45236 (9)	0.0375 (4)

H12A	0.5627	−0.1555	0.4258	0.045*
H12B	0.5966	−0.0851	0.4995	0.045*
C13	0.76758 (16)	−0.15711 (12)	0.47099 (8)	0.0294 (3)
C14	0.88512 (18)	−0.11324 (14)	0.44907 (9)	0.0379 (4)
H14	0.8783	−0.0491	0.4214	0.046*
C15	1.01216 (19)	−0.16348 (15)	0.46771 (11)	0.0478 (5)
H15	1.0900	−0.1343	0.4517	0.057*
C16	1.02296 (19)	−0.25688 (16)	0.51008 (11)	0.0488 (5)
H16	1.1089	−0.2898	0.5239	0.059*
C17	0.90668 (18)	−0.30224 (14)	0.53235 (9)	0.0409 (4)
H17	0.9148	−0.3657	0.5608	0.049*
C18	0.77854 (16)	−0.25356 (12)	0.51251 (8)	0.0304 (3)
C19	0.64901 (18)	−0.30062 (13)	0.53515 (10)	0.0426 (4)
H19A	0.6259	−0.2593	0.5775	0.051*
H19B	0.5732	−0.2925	0.4930	0.051*
C20	0.64394 (19)	−0.45501 (12)	0.62419 (8)	0.0382 (4)
H20	0.6285	−0.4133	0.6653	0.046*
C21	0.67567 (18)	−0.58996 (13)	0.55355 (9)	0.0407 (4)
H21	0.6869	−0.6603	0.5371	0.049*
C22	0.67997 (19)	−0.50032 (14)	0.51112 (9)	0.0433 (4)
H22	0.6934	−0.4972	0.4608	0.052*
O1	0.69190 (13)	0.35191 (9)	0.11146 (6)	0.0465 (3)
O2	0.69910 (18)	0.28649 (10)	0.22607 (7)	0.0728 (5)
O3	0.63128 (16)	0.76656 (10)	0.24541 (8)	0.0623 (4)
O4	0.61815 (14)	0.65379 (10)	0.33933 (7)	0.0507 (3)
Co1	0.58188 (3)	0.163209 (16)	0.199462 (11)	0.03716 (9)
N1	0.61394 (14)	0.09605 (10)	0.30478 (7)	0.0355 (3)
N2	0.62601 (13)	−0.00679 (10)	0.40605 (6)	0.0320 (3)
N3	0.66068 (14)	−0.41468 (10)	0.55676 (7)	0.0363 (3)
N4	0.65211 (15)	−0.56183 (10)	0.62477 (7)	0.0376 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0446 (10)	0.0288 (8)	0.0349 (8)	0.0005 (7)	0.0134 (7)	−0.0012 (7)
C2	0.0450 (10)	0.0350 (9)	0.0322 (8)	−0.0061 (8)	0.0081 (7)	−0.0004 (7)
C3	0.0651 (13)	0.0405 (9)	0.0284 (8)	−0.0088 (9)	0.0029 (8)	0.0044 (7)
C4	0.0632 (13)	0.0539 (11)	0.0357 (9)	−0.0103 (10)	0.0036 (9)	−0.0056 (8)
C5	0.0629 (13)	0.0392 (9)	0.0427 (10)	−0.0196 (9)	0.0144 (9)	−0.0098 (8)
C6	0.0732 (15)	0.0381 (10)	0.0474 (10)	−0.0159 (9)	0.0239 (10)	−0.0020 (8)
C7	0.0710 (14)	0.0358 (9)	0.0299 (8)	−0.0082 (9)	0.0136 (8)	0.0033 (7)
C8	0.0704 (14)	0.0320 (8)	0.0376 (9)	−0.0129 (9)	0.0144 (9)	−0.0138 (8)
C9	0.0589 (12)	0.0271 (8)	0.0317 (8)	−0.0047 (8)	0.0065 (8)	−0.0034 (7)
C10	0.0442 (10)	0.0390 (9)	0.0261 (7)	−0.0042 (8)	0.0028 (7)	−0.0037 (7)
C11	0.0484 (11)	0.0268 (7)	0.0267 (7)	−0.0009 (7)	0.0057 (7)	−0.0001 (6)
C12	0.0350 (10)	0.0401 (9)	0.0376 (8)	−0.0006 (7)	0.0064 (7)	0.0152 (7)
C13	0.0305 (9)	0.0332 (8)	0.0241 (7)	−0.0033 (7)	0.0036 (6)	0.0005 (6)
C14	0.0377 (10)	0.0389 (9)	0.0377 (8)	−0.0064 (8)	0.0077 (7)	0.0040 (7)

C15	0.0334 (11)	0.0568 (11)	0.0551 (11)	−0.0066 (9)	0.0132 (9)	−0.0003 (9)
C16	0.0302 (11)	0.0564 (11)	0.0590 (11)	0.0073 (9)	0.0050 (8)	−0.0021 (9)
C17	0.0405 (11)	0.0386 (9)	0.0421 (9)	0.0045 (8)	0.0023 (8)	0.0042 (8)
C18	0.0327 (9)	0.0321 (8)	0.0264 (7)	−0.0001 (7)	0.0052 (6)	0.0009 (6)
C19	0.0405 (11)	0.0357 (8)	0.0533 (10)	0.0041 (8)	0.0127 (8)	0.0184 (8)
C20	0.0537 (11)	0.0320 (8)	0.0305 (8)	0.0004 (8)	0.0114 (7)	0.0034 (7)
C21	0.0508 (11)	0.0338 (8)	0.0413 (9)	−0.0012 (8)	0.0187 (8)	−0.0043 (7)
C22	0.0542 (12)	0.0466 (10)	0.0337 (8)	−0.0053 (9)	0.0201 (8)	−0.0009 (8)
O1	0.0559 (8)	0.0480 (7)	0.0332 (6)	−0.0070 (6)	0.0002 (6)	−0.0032 (5)
O2	0.1385 (15)	0.0422 (7)	0.0405 (7)	−0.0395 (9)	0.0230 (8)	−0.0041 (6)
O3	0.0897 (11)	0.0376 (7)	0.0610 (8)	0.0019 (7)	0.0166 (8)	0.0034 (6)
O4	0.0642 (9)	0.0535 (8)	0.0360 (6)	−0.0124 (6)	0.0131 (6)	−0.0060 (5)
Co1	0.06634 (19)	0.02305 (11)	0.02269 (11)	−0.00140 (10)	0.00917 (10)	−0.00115 (8)
N1	0.0525 (9)	0.0282 (7)	0.0257 (6)	−0.0011 (6)	0.0065 (6)	0.0003 (5)
N2	0.0348 (8)	0.0334 (7)	0.0274 (6)	−0.0003 (6)	0.0037 (5)	0.0080 (5)
N3	0.0443 (9)	0.0333 (7)	0.0331 (6)	−0.0007 (6)	0.0115 (6)	0.0086 (6)
N4	0.0510 (9)	0.0309 (7)	0.0317 (7)	0.0005 (6)	0.0089 (6)	0.0037 (6)

Geometric parameters (Å, º)

C1—O1	1.2240 (19)	C12—C13	1.503 (2)
C1—O2	1.2673 (19)	C12—H12A	0.9700
C1—C2	1.524 (2)	C12—H12B	0.9700
C2—C7	1.531 (2)	C13—C14	1.385 (2)
C2—C3	1.538 (2)	C13—C18	1.398 (2)
C2—H2	0.9800	C14—C15	1.380 (2)
C3—C4	1.521 (2)	C14—H14	0.9300
C3—H3A	0.9700	C15—C16	1.374 (3)
C3—H3B	0.9700	C15—H15	0.9300
C4—C5	1.527 (3)	C16—C17	1.385 (3)
C4—H4A	0.9700	C16—H16	0.9300
C4—H4B	0.9700	C17—C18	1.383 (2)
C5—C8	1.526 (3)	C17—H17	0.9300
C5—C6	1.536 (3)	C18—C19	1.509 (2)
C5—H5	0.9800	C19—N3	1.461 (2)
C6—C7	1.527 (2)	C19—H19A	0.9700
C6—H6A	0.9700	C19—H19B	0.9700
C6—H6B	0.9700	C20—N4	1.3222 (19)
C7—H7A	0.9700	C20—N3	1.3377 (19)
C7—H7B	0.9700	C20—H20	0.9300
C8—O3	1.237 (2)	C21—C22	1.346 (2)
C8—O4	1.289 (2)	C21—N4	1.374 (2)
C9—C10	1.345 (2)	C21—H21	0.9300
C9—N1	1.376 (2)	C22—N3	1.367 (2)
C9—H9	0.9300	C22—H22	0.9300
C10—N2	1.367 (2)	O2—Co1	1.9185 (13)
C10—H10	0.9300	O4—Co1^{i}	1.9682 (15)
C11—N1	1.3199 (19)	Co1—O4^{ii}	1.9682 (15)

C11—N2	1.3432 (18)	Co1—N4^{iii}	2.0306 (13)
C11—H11	0.9300	Co1—N1	2.0311 (12)
C12—N2	1.4541 (19)	N4—Co1^{iv}	2.0306 (13)
O1—C1—O2	123.04 (15)	C13—C12—H12B	108.7
O1—C1—C2	121.85 (14)	H12A—C12—H12B	107.6
O2—C1—C2	115.09 (14)	C14—C13—C18	119.29 (15)
C1—C2—C7	111.52 (13)	C14—C13—C12	122.16 (14)
C1—C2—C3	111.46 (13)	C18—C13—C12	118.55 (14)
C7—C2—C3	111.64 (13)	C15—C14—C13	120.84 (16)
C1—C2—H2	107.3	C15—C14—H14	119.6
C7—C2—H2	107.3	C13—C14—H14	119.6
C3—C2—H2	107.3	C16—C15—C14	119.63 (17)
C4—C3—C2	113.23 (14)	C16—C15—H15	120.2
C4—C3—H3A	108.9	C14—C15—H15	120.2
C2—C3—H3A	108.9	C15—C16—C17	120.41 (17)
C4—C3—H3B	108.9	C15—C16—H16	119.8
C2—C3—H3B	108.9	C17—C16—H16	119.8
H3A—C3—H3B	107.7	C18—C17—C16	120.26 (16)
C3—C4—C5	111.62 (14)	C18—C17—H17	119.9
C3—C4—H4A	109.3	C16—C17—H17	119.9
C5—C4—H4A	109.3	C17—C18—C13	119.54 (15)
C3—C4—H4B	109.3	C17—C18—C19	122.00 (14)
C5—C4—H4B	109.3	C13—C18—C19	118.46 (14)
H4A—C4—H4B	108.0	N3—C19—C18	114.22 (14)
C8—C5—C4	114.75 (16)	N3—C19—H19A	108.7
C8—C5—C6	110.77 (16)	C18—C19—H19A	108.7
C4—C5—C6	108.75 (15)	N3—C19—H19B	108.7
C8—C5—H5	107.4	C18—C19—H19B	108.7
C4—C5—H5	107.4	H19A—C19—H19B	107.6
C6—C5—H5	107.4	N4—C20—N3	111.26 (14)
C7—C6—C5	110.70 (14)	N4—C20—H20	124.4
C7—C6—H6A	109.5	N3—C20—H20	124.4
C5—C6—H6A	109.5	C22—C21—N4	109.76 (14)
C7—C6—H6B	109.5	C22—C21—H21	125.1
C5—C6—H6B	109.5	N4—C21—H21	125.1
H6A—C6—H6B	108.1	C21—C22—N3	106.33 (14)
C6—C7—C2	112.53 (14)	C21—C22—H22	126.8
C6—C7—H7A	109.1	N3—C22—H22	126.8
C2—C7—H7A	109.1	C1—O2—Co1	125.78 (11)
C6—C7—H7B	109.1	C8—O4—Co1^{i}	109.44 (12)
C2—C7—H7B	109.1	O2—Co1—O4^{ii}	130.75 (6)
H7A—C7—H7B	107.8	O2—Co1—N4^{iii}	113.50 (6)
O3—C8—O4	121.2 (2)	O4^{ii}—Co1—N4^{iii}	99.08 (6)
O3—C8—C5	120.01 (17)	O2—Co1—N1	95.80 (5)
O4—C8—C5	118.80 (17)	O4^{ii}—Co1—N1	107.05 (5)
C10—C9—N1	109.56 (14)	N4^{iii}—Co1—N1	109.79 (5)
C10—C9—H9	125.2	C11—N1—C9	105.55 (12)

N1—C9—H9	125.2	C11—N1—Co1	133.27 (10)
C9—C10—N2	106.62 (13)	C9—N1—Co1	121.00 (10)
C9—C10—H10	126.7	C11—N2—C10	107.12 (12)
N2—C10—H10	126.7	C11—N2—C12	125.77 (13)
N1—C11—N2	111.14 (13)	C10—N2—C12	127.07 (12)
N1—C11—H11	124.4	C20—N3—C22	107.30 (13)
N2—C11—H11	124.4	C20—N3—C19	125.54 (14)
N2—C12—C13	114.42 (13)	C22—N3—C19	127.00 (13)
N2—C12—H12A	108.7	C20—N4—C21	105.34 (13)
C13—C12—H12A	108.7	C20—N4—Co1^{iv}	126.46 (11)
N2—C12—H12B	108.7	C21—N4—Co1^{iv}	125.35 (11)

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