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Crystal structure of tris[hexakis(imidazole)-cobalt(II)] bis(benzene-1,3,5-tricarboxylate)

Jose de Jesus Velazquez-Garcia,[a]* Christos Bintas,[a,b] Faegheh Khademhir,[a,c] Bassima Knjo,[a,c] Aliyenur Ekineken,[a,c] Fabienne Hain[a,c] and Simone Techert[a,d]

[a]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany, [b]Department of Chemistry, National and Kapodistrian University of Athens (NKUA), Zografou 157 72, Greece, [c]BS 06 Berufliche Schule Chemie, Biologie, Pharmazie, Agrarwirtschaft, Ladenbeker, Furtweg 151, 21033 Hamburg, Germany, and [d]Institut für Röntgenphysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany. *Correspondence e-mail: jose.velazquez@desy.de

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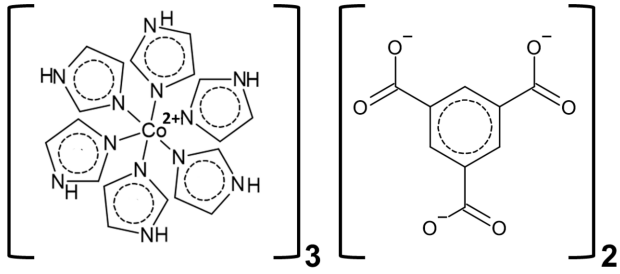
The title compound, $[Co^{II}(C_3H_4N_2)_6]_3(C_9H_3O_6)_2$ (**1**), was synthesized from cobalt chloride(II), benzene-1,3,5-tricarboxylic acid (H_3btc) and imidazole (Im) in an ethanol/DMF mixture *via* slow evaporation at room temperature. This compound consists of three hexakis(imidazole)cobalt(II) cations and two trimesate anions. Examination of the crystal packing shows the formation of one-dimensional stacks of ions propagating along the *c* axis. The packing interactions are primarily driven by N—H···O hydrogen bonding between anions and cations.

1. Chemical context

Benzene-1,3,5-tricarboxylic acid (trimesic acid, H_3btc) and imidazole derivatives are typically used in the synthesis of metal–organic frameworks (MOFs). For example, imidazole (Im) and 2-methylimidazole (2mIm) serve as ligands in the synthesis of the reported zeolitic imidazolate frameworks ZIF-4 and ZIF-8, respectively (Park *et al.*, 2006). Likewise, H_3btc is a key precursor in the synthesis of the well-known MOFs MIL-100 (Férey *et al.*, 2004) and HKUST-1 (Chui *et al.*, 1999). In previous work, we have employed 2-methylimidazole and H_3btc to synthesize a small coordination complex (Velazquez-Garcia & Techert, 2022), various organic salts (Baletska *et al.*, 2023; Asprilla-Herrera *et al.*, 2025; Łukaszczyk *et al.*, 2025) and two mixed-ligand MOFs (Velazquez Garcia *et al.*, 2025). In the present study, we substituted 2-methylimidazole with imidazole to synthesize the title compound (**1**).



2. Structural commentary

Compound **1** (Fig. 1) crystallizes in the trigonal $R\overline{3}$ space group. The complete group contains three hexakis(imidazole)cobalt(II) cations and two fully deprotonated btc^{3-} anions. The asymmetric unit comprises one third of a

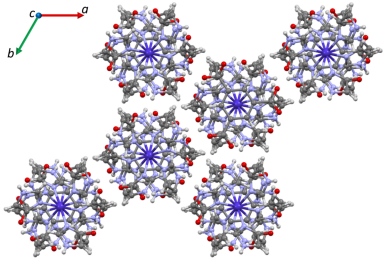


Table 1
Hydrogen-bond geometry (Å,°).

D—H···A	Type	Graph-set	D—H	H···A	D···A	D—H···A
N4—H4···O1	*a*	$DR^2_2(16)$	0.856 (14)	1.908 (14)	2.7282 (17)	160.0 (4)
N2—H2···O1^{i}	*b*	$DC^2_2(16)R^6_6(48)$	0.835 (13)	1.991 (13)	2.7661 (18)	154.0 (12)
N6—H6*A*···O2	*c*	$DR^2_2(16)$	0.841 (14)	2.075 (12)	2.8161 (17)	146.8 (4)
N6—H6*A*···O2^{ii}	*d*	$DC^2_2(16)R^4_4(32)R^6_6(48)$	0.841 (14)	2.446 (9)	3.0298 (17)	127.2 (3)

Symmetry codes: (i) $\frac{2}{3} - x + y$, $4/3 - x$, $\frac{1}{3} + z$; (ii) $4/3 - x$, $\frac{5}{3} - y$, $\frac{2}{3} - z$.

btc^{3-} anion and two crystallographically independent metal centres (Co1 and Co2) – one third of Co1 coordinated by two Im ligands and one sixth of Co2 coordinated by a single Im ligand. Both metal centres and the centre of mass of the btc^{3-} ion lie on the $\overline{3}$ rotoinversion axis, while Co2 is located exactly on the inversion centre.

To estimate the distortion from the ideal octahedral geometry of the cations, the parameters Σ (Halcrow, 2011) and Θ (Marchivie *et al.*, 2005) were calculated using the *OctaDist* program (Ketkaew *et al.*, 2021). While Σ summarizes the deviation of the N—Co—N angles from 90°, Θ indicates the degree of twist from a perfect octahedron towards a trigonal prism. In an ideal octahedron, both parameters are equal to zero, whereas Θ reaches 1140° for a perfect trigonal prism. The calculated values of the distortion parameters Σ/Θ for Co1 and Co2 are equal to 13°/27° and 10°/23°, respectively. Both parameters exhibit a slight distortion of the coordination environment of both metal centres.

3. Supramolecular features

Crystal packing diagrams of compound **1** as viewed down the *c* and *a* axes are shown in Figs. 2 and 3, respectively. The figures show columns of ions stacked along the *c* axis, following a repeating polar arrangement: anion – cation – cation – anion – cation. Each column interacts with others *via* hydrogen bonding of the N—H···O type (Fig. 3), summarized in Table 1. The table demonstrates that all possible donor and acceptor groups are involved in moderate hydrogen bonds. The presence of different hydrogen bonds in **1** results in characteristic arrays that may be described by graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995)**.** In the structure of **1**, there are ten motifs involved in discrete *D* (all types), ring *R* (all types) and chains *C* (types *b* and *d*). Notably, hydrogen bonds *b* and *d* hold the aforementioned columns together, whereas *a* and *c* strengthen the interaction between ions within the columns.

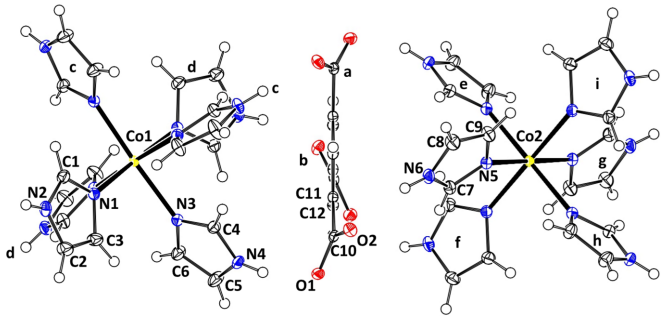


Figure 1
Crystal structure of **1** with displacement ellipsoids drawn at the 50% probability level. Atoms labelled by group are generated by the following symmetry operations: $1 - y$, $1 + x - y$, z for groups a, c and e; $-x + y$, $1 - x$, z for groups b, d and f; $\frac{2}{3} - x$, $\frac{4}{3} - y$, $\frac{1}{3} - z$ for fractions g and i; $-\frac{1}{3} + y$, $\frac{1}{3} - x + y$, $\frac{1}{3} - z$ for group h.

4. Database survey

No reported structures of the title compound were found in the Cambridge Structural Database (CSD version 5.45, update of November 2023; Groom *et al.*, 2016). Some structures containing the hexakis(imidazole)cobalt(II) cation and polycarboxylate anions were reported under the refcodes AGAXIS (Jyai & Srinivasan, 2019), BOVMIJ (Nie *et al.*, 2009)

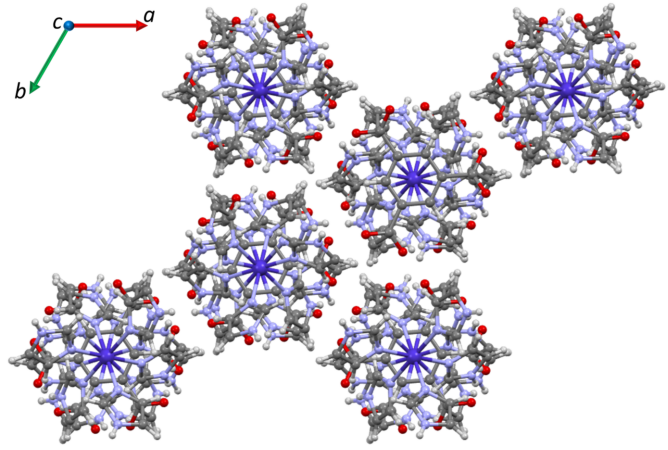


Figure 2
Packing diagram of **1** down the *c* axis.

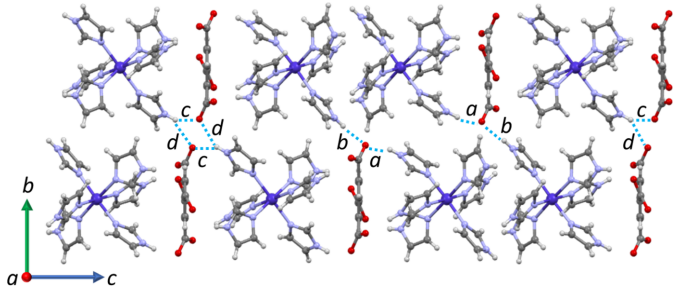


Figure 3
Crystal packing of **1** viewed along the *a* axis, showing only two representative stacks for clarity. Only discrete graph-set motifs are highlighted (*a*–*d*).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(C_3H_4N_2)_6]_3(C_9H_3O_6)_2$
M_r	1816.49
Crystal system, space group	Trigonal, $R\overline{3}$
Temperature (K)	100
a, c (Å)	15.215 (2), 30.494 (6)
V (Å^3)	6113 (2)
Z	3
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.69
Crystal size (mm)	0.6 × 0.4 × 0.2
Data collection	
Diffractometer	Bruker P4
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.690, 0.748
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28365, 3380, 3106
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.076, 1.04
No. of reflections	3380
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.33

Computer programs: *APEX2* and *APEX2* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

and EFIVOE (Tong *et al.*, 2002). However, none of them include btc^{3-} as counter-ion but benzene-1,2-dicarboxylate, bis(naphthalene-1,4-dicarboxylate) and 1,4-benzenedicarboxylate, respectively.

5. Synthesis and crystallization

In a typical synthesis, 100 µL of a 0.11 *M* ethanolic solution of $CoCl_2{\cdot}6H_2O$ was diluted with 100 µL of *N*,*N*-dimethylformamide, followed by the addition of 120 µL of a 1.58 *M* ethanolic solution of imidazole. Then, 100 µL of a 0.12 *M* ethanolic solution of H_3btc was added to the mixture. The resulting mixture was gently shaken and allowed to dry slowly at room temperature. After three weeks, red crystals of **1** were obtained.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The positions of hydrogen atoms were refined with U_{iso}(H) = 1.2U_{eq}(C or N) for CH and NH groups. Hydrogen atoms bonded to nitrogen atoms (N—H) were treated with free refinement of bond distances. The most disagreeable reflections ($\overline{4}$50 and 244) with error/s.u. of more than ten were omitted using the OMIT instruction in *SHELXL* (Sheldrick, 2015*b*).

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Crystal structure of tris[hexakis(imidazole)cobalt(II)] bis(benzene-1,3,5-tricarboxylate)

Jose de Jesus Velazquez-Garcia, Christos Bintas, Faegheh Khademhir, Bassima Knjo, Aliyenur Ekineken, Fabienne Hain and Simone Techert

Computing details

Tris[hexakis(imidazole)cobalt(II)] bis(benzene-1,3,5-tricarboxylate)

Crystal data

$[Co(C_3H_4N_2)_6]_3(C_9H_3O_6)_2$
M_r = 1816.49
Trigonal, $R\overline{3}$
a = 15.215 (2) Å
c = 30.494 (6) Å
V = 6113 (2) Å^3
Z = 3
$F(000)$ = 2817
D_x = 1.480 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9869 reflections
θ = 2.7–39.6°
μ = 0.69 mm^{-1}
T = 100 K
Rhombohedral, red
0.6 × 0.4 × 0.2 mm

Data collection

Bruker P4 diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.690, T_{max} = 0.748
28365 measured reflections
3380 independent reflections
3106 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 28.3°, θ_{min} = 1.7°
h = −20→20
k = −20→20
l = −40→40
Standard reflections: not measured; every not measured reflections
intensity decay: not measured

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.076
S = 1.04
3380 reflections
199 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 12.840P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.333333	0.666667	0.55111 (2)	0.00919 (8)
Co2	0.333333	0.666667	0.166667	0.00965 (10)
O2	0.59402 (7)	0.71916 (7)	0.34095 (3)	0.01540 (19)
O1	0.50598 (7)	0.56614 (7)	0.37221 (3)	0.01563 (19)
N1	0.46175 (8)	0.69448 (8)	0.59020 (3)	0.0127 (2)
N3	0.35884 (8)	0.56677 (8)	0.50903 (3)	0.0129 (2)
N5	0.46325 (8)	0.75844 (8)	0.20837 (3)	0.0131 (2)
N4	0.40359 (9)	0.51431 (9)	0.44997 (4)	0.0165 (2)
H4	0.4338 (7)	0.51618 (10)	0.4260 (5)	0.020*
N2	0.58846 (8)	0.75732 (9)	0.63733 (4)	0.0160 (2)
H2	0.6292 (9)	0.7952 (9)	0.6564 (4)	0.019*
N6	0.56893 (9)	0.80854 (9)	0.26463 (4)	0.0163 (2)
H6A	0.5978 (7)	0.80585 (11)	0.2877 (5)	0.020*
C11	0.42044 (9)	0.65755 (9)	0.35769 (4)	0.0121 (2)
C12	0.32434 (9)	0.57106 (9)	0.35767 (4)	0.0128 (2)
H12	0.31828 (15)	0.5068 (12)	0.35765 (4)	0.015*
C10	0.51488 (9)	0.64817 (9)	0.35684 (4)	0.0122 (2)
C4	0.41613 (10)	0.59442 (10)	0.47339 (4)	0.0153 (2)
H4A	0.4609 (9)	0.6629 (13)	0.46533 (16)	0.018*
C7	0.49165 (10)	0.72946 (10)	0.24412 (4)	0.0152 (2)
H7	0.4615 (6)	0.6621 (13)	0.25389 (19)	0.018*
C1	0.51171 (10)	0.76558 (10)	0.61989 (4)	0.0170 (2)
H1	0.4959 (3)	0.8149 (10)	0.62771 (16)	0.020*
C9	0.52659 (10)	0.86245 (10)	0.20645 (4)	0.0184 (3)
H9	0.52491 (11)	0.9039 (9)	0.1851 (4)	0.022*
C8	0.59212 (11)	0.89424 (11)	0.24123 (5)	0.0202 (3)
H8	0.6424 (10)	0.9607 (14)	0.24769 (14)	0.024*
C2	0.58792 (11)	0.67609 (11)	0.61821 (5)	0.0211 (3)
H2A	0.6330 (9)	0.6514 (5)	0.62393 (13)	0.025*
C3	0.50915 (11)	0.63748 (11)	0.58913 (5)	0.0201 (3)
H3	0.4896 (4)	0.5789 (12)	0.5706 (4)	0.024*
C6	0.30649 (11)	0.46203 (10)	0.50802 (4)	0.0200 (3)
H6	0.2597 (10)	0.4201 (9)	0.5291 (4)	0.024*
C5	0.33334 (12)	0.42898 (11)	0.47158 (5)	0.0243 (3)
H5	0.3089 (5)	0.3622 (15)	0.46314 (19)	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.00977 (10)	0.00977 (10)	0.00803 (13)	0.00488 (5)	0.000	0.000
Co2	0.01060 (13)	0.01060 (13)	0.00775 (18)	0.00530 (6)	0.000	0.000
O2	0.0124 (4)	0.0163 (4)	0.0162 (4)	0.0061 (4)	−0.0005 (3)	0.0012 (3)
O1	0.0194 (4)	0.0169 (4)	0.0148 (4)	0.0122 (4)	0.0048 (3)	0.0028 (3)
N1	0.0134 (5)	0.0136 (5)	0.0114 (5)	0.0069 (4)	0.0001 (4)	0.0005 (4)
N3	0.0138 (5)	0.0136 (5)	0.0121 (5)	0.0074 (4)	−0.0003 (4)	−0.0004 (4)
N5	0.0135 (5)	0.0142 (5)	0.0114 (5)	0.0067 (4)	−0.0001 (4)	−0.0002 (4)
N4	0.0216 (6)	0.0174 (5)	0.0128 (5)	0.0116 (5)	0.0047 (4)	0.0000 (4)
N2	0.0133 (5)	0.0196 (5)	0.0125 (5)	0.0062 (4)	−0.0026 (4)	−0.0019 (4)
N6	0.0161 (5)	0.0218 (6)	0.0118 (5)	0.0101 (5)	−0.0037 (4)	−0.0026 (4)
C11	0.0132 (5)	0.0151 (6)	0.0093 (5)	0.0080 (5)	0.0003 (4)	0.0000 (4)
C12	0.0153 (6)	0.0127 (6)	0.0109 (5)	0.0074 (5)	−0.0005 (4)	−0.0003 (4)
C10	0.0139 (5)	0.0150 (6)	0.0091 (5)	0.0082 (5)	−0.0012 (4)	−0.0030 (4)
C4	0.0167 (6)	0.0143 (6)	0.0151 (6)	0.0079 (5)	0.0023 (5)	0.0002 (5)
C7	0.0150 (6)	0.0174 (6)	0.0131 (6)	0.0080 (5)	−0.0008 (4)	0.0003 (4)
C1	0.0175 (6)	0.0205 (6)	0.0148 (6)	0.0109 (5)	−0.0021 (5)	−0.0039 (5)
C9	0.0191 (6)	0.0149 (6)	0.0171 (6)	0.0053 (5)	−0.0035 (5)	0.0009 (5)
C8	0.0190 (6)	0.0166 (6)	0.0204 (6)	0.0055 (5)	−0.0053 (5)	−0.0022 (5)
C2	0.0182 (6)	0.0241 (7)	0.0246 (7)	0.0133 (6)	−0.0062 (5)	−0.0036 (5)
C3	0.0201 (6)	0.0211 (7)	0.0238 (7)	0.0138 (6)	−0.0074 (5)	−0.0060 (5)
C6	0.0262 (7)	0.0140 (6)	0.0179 (6)	0.0087 (5)	0.0081 (5)	0.0017 (5)
C5	0.0334 (8)	0.0139 (6)	0.0228 (7)	0.0098 (6)	0.0106 (6)	0.0000 (5)

Geometric parameters (Å, º)

Co1—N1	2.1426 (11)	N2—H2	0.836 (19)
Co1—N1^{i}	2.1426 (11)	N2—C1	1.3448 (17)
Co1—N1^{ii}	2.1426 (11)	N2—C2	1.3629 (18)
Co1—N3	2.1673 (11)	N6—H6A	0.840 (19)
Co1—N3^{ii}	2.1673 (11)	N6—C7	1.3441 (17)
Co1—N3^{i}	2.1673 (11)	N6—C8	1.3689 (18)
Co2—N5^{iii}	2.1710 (11)	C11—C12^{i}	1.3965 (17)
Co2—N5^{ii}	2.1712 (11)	C11—C12	1.3948 (17)
Co2—N5	2.1711 (11)	C11—C10	1.5136 (17)
Co2—N5^{iv}	2.1711 (11)	C12—H12	0.935 (18)
Co2—N5^{i}	2.1711 (11)	C4—H4A	0.949 (18)
Co2—N5^{v}	2.1711 (11)	C7—H7	0.938 (18)
O2—C10	1.2452 (16)	C1—H1	0.927 (18)
O1—C10	1.2755 (15)	C9—H9	0.917 (19)
N1—C1	1.3212 (17)	C9—C8	1.3679 (18)
N1—C3	1.3780 (17)	C8—H8	0.935 (19)
N3—C4	1.3233 (16)	C2—H2A	0.948 (19)
N3—C6	1.3805 (17)	C2—C3	1.3652 (19)
N5—C7	1.3269 (16)	C3—H3	0.968 (19)
N5—C9	1.3826 (17)	C6—H6	0.935 (19)

N4—H4	0.855 (18)	C6—C5	1.3637 (19)
N4—C4	1.3413 (17)	C5—H5	0.93 (2)
N4—C5	1.3690 (18)		

N1—Co1—N1^{i}	92.04 (4)	C1—N2—H2	126.2
N1—Co1—N1^{ii}	92.04 (4)	C1—N2—C2	107.69 (11)
N1^{i}—Co1—N1^{ii}	92.04 (4)	C2—N2—H2	126.2
N1^{i}—Co1—N3^{ii}	89.24 (4)	C7—N6—H6A	126.2
N1^{ii}—Co1—N3^{i}	177.42 (4)	C7—N6—C8	107.68 (11)
N1—Co1—N3^{i}	89.24 (4)	C8—N6—H6A	126.2
N1^{ii}—Co1—N3^{ii}	90.15 (4)	C12—C11—C12^{i}	119.40 (12)
N1—Co1—N3	90.15 (4)	C12—C11—C10	120.52 (11)
N1^{i}—Co1—N3^{i}	90.15 (4)	C12^{i}—C11—C10	120.07 (11)
N1^{i}—Co1—N3	177.42 (4)	C11—C12—C11^{ii}	120.60 (12)
N1^{ii}—Co1—N3	89.24 (4)	C11—C12—H12	119.7
N1—Co1—N3^{ii}	177.42 (4)	C11^{ii}—C12—H12	119.7
N3—Co1—N3^{i}	88.52 (4)	O2—C10—O1	125.12 (11)
N3—Co1—N3^{ii}	88.52 (4)	O2—C10—C11	118.48 (11)
N3^{ii}—Co1—N3^{i}	88.52 (4)	O1—C10—C11	116.40 (11)
N5^{iii}—Co2—N5^{iv}	89.17 (4)	N3—C4—N4	112.12 (12)
N5^{v}—Co2—N5	90.83 (4)	N3—C4—H4A	123.9
N5^{v}—Co2—N5^{ii}	180.00 (6)	N4—C4—H4A	123.9
N5^{iii}—Co2—N5^{i}	180.0	N5—C7—N6	111.68 (12)
N5^{iv}—Co2—N5^{ii}	90.83 (4)	N5—C7—H7	124.2
N5^{iv}—Co2—N5^{i}	90.83 (4)	N6—C7—H7	124.2
N5^{i}—Co2—N5	89.17 (4)	N1—C1—N2	111.44 (12)
N5^{iii}—Co2—N5^{v}	89.17 (4)	N1—C1—H1	124.3
N5^{iii}—Co2—N5^{ii}	90.83 (4)	N2—C1—H1	124.3
N5^{iv}—Co2—N5^{v}	89.17 (4)	N5—C9—H9	125.1
N5^{i}—Co2—N5^{ii}	89.17 (4)	C8—C9—N5	109.85 (12)
N5^{iii}—Co2—N5	90.83 (4)	C8—C9—H9	125.1
N5—Co2—N5^{ii}	89.17 (4)	N6—C8—H8	127.1
N5^{iv}—Co2—N5	180.00 (4)	C9—C8—N6	105.80 (12)
N5^{i}—Co2—N5^{v}	90.83 (4)	C9—C8—H8	127.1
C1—N1—Co1	129.61 (9)	N2—C2—H2A	127.1
C1—N1—C3	105.28 (11)	N2—C2—C3	105.89 (12)
C3—N1—Co1	125.11 (9)	C3—C2—H2A	127.1
C4—N3—Co1	125.72 (9)	N1—C3—H3	125.2
C4—N3—C6	104.88 (11)	C2—C3—N1	109.70 (12)
C6—N3—Co1	128.35 (9)	C2—C3—H3	125.2
C7—N5—Co2	127.63 (9)	N3—C6—H6	125.1
C7—N5—C9	105.00 (11)	C5—C6—N3	109.72 (12)
C9—N5—Co2	126.92 (9)	C5—C6—H6	125.1
C4—N4—H4	126.4	N4—C5—H5	126.9
C4—N4—C5	107.12 (11)	C6—C5—N4	106.16 (12)
C5—N4—H4	126.4	C6—C5—H5	126.9

Co1—N1—C1—N2	179.95 (8)	C10—C11—C12—C11^{ii}	−178.88 (8)

Co1—N1—C3—C2	−179.87 (10)	C4—N3—C6—C5	−0.21 (16)
Co1—N3—C4—N4	−169.11 (8)	C4—N4—C5—C6	−0.41 (17)
Co1—N3—C6—C5	168.45 (10)	C7—N5—C9—C8	−0.03 (16)
Co2—N5—C7—N6	−172.93 (8)	C7—N6—C8—C9	−0.42 (15)
Co2—N5—C9—C8	172.72 (9)	C1—N1—C3—C2	−0.46 (16)
N3—C6—C5—N4	0.39 (18)	C1—N2—C2—C3	0.16 (16)
N5—C9—C8—N6	0.28 (16)	C9—N5—C7—N6	−0.24 (15)
N2—C2—C3—N1	0.18 (17)	C8—N6—C7—N5	0.42 (15)
C12^{i}—C11—C12—C11^{ii}	−0.1 (2)	C2—N2—C1—N1	−0.47 (16)
C12^{i}—C11—C10—O2	−25.08 (17)	C3—N1—C1—N2	0.57 (15)
C12—C11—C10—O2	153.71 (12)	C6—N3—C4—N4	−0.05 (15)
C12—C11—C10—O1	−25.38 (17)	C5—N4—C4—N3	0.30 (16)
C12^{i}—C11—C10—O1	155.82 (11)		

Symmetry codes: (i) −*y*+1, *x*−*y*+1, *z*; (ii) −*x*+*y*, −*x*+1, *z*; (iii) *y*−1/3, −*x*+*y*+1/3, −*z*+1/3; (iv) −*x*+2/3, −*y*+4/3, −*z*+1/3; (v) *x*−*y*+2/3, *x*+1/3, −*z*+1/3.