

## Retraction of articles

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This article reports the retraction of 11 articles published in *Acta Crystallographica Section E* between 2005 and 2009.

After further thorough investigation (see Harrison *et al.*, 2010), 11 additional articles are retracted by the authors or by the journal as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

**Table 1**

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
[ <i>N,N'</i> -Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)	Chen <i>et al.</i> (2005)	10.1107/S1600536805026796	YAWZOM
Diazidobis(2,2'-biimidazole)copper(II)	Liu <i>et al.</i> (2007)	10.1107/S1600536807047873	SILZIX
Dichlorido(1,10-phenanthroline)copper(II)	Liu (2007)	10.1107/S1600536807056735	MISSAJ
Diazidobis(2,2'-biimidazole)cobalt(II)	Li <i>et al.</i> (2008)	10.1107/S1600536807062873	MIRYAO
Diazidobis(2,2'-biimidazole)manganese(II)	Zhang <i>et al.</i> (2008)	10.1107/S1600536808017984	MODBUD
Diazidobis(2,2'-biimidazole)iron(II)	Hao <i>et al.</i> (2008a)	10.1107/S1600536808018539	MODFOB
Bis(pentane-2,4-dionato)bis[2-(4-pyridyl)-4,4,5,5-tetramethylimidazoline-1-oxyl 3-oxide]nickel(II)	Hao <i>et al.</i> (2008b)	10.1107/S1600536808018552	MODFUH
Bis(pentane-2,4-dionato- $\kappa^2 O, O'$ )bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide- $\kappa^2 N^2$ ]manganese(II)	Liu, Zhang <i>et al.</i> (2008)	10.1107/S1600536808022952	MODLUN
Bis[2,4-pentanedionato(1-)]bis[4,4,5,5-tetramethyl-2-(4-pyridyl)imidazoline-1-oxyl 3-oxide]manganese(II)	Liu, He <i>et al.</i> (2008)	10.1107/S1600536808038440	MODLUN01
Di- $\mu$ -chlorido-bis[chlorido(1,10-phenanthroline- $\kappa^2 N, N'$ )zinc(II)]	Yang <i>et al.</i> (2009)	10.1107/S1600536809014482	JOLBOC
Tris(ethylenediamine)manganese(II) sulfate	Lu (2009)	10.1107/S1600536809034874	YUCZEC

## References

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- Hao, L., Mu, C. & Kong, B. (2008b). *Acta Cryst.* **E64**, m957.
- Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* **E66**, e1–e2.
- Li, S., Wang, S.-B., Zhang, F.-L. & Tang, K. (2008). *Acta Cryst.* **E64**, m76.
- Liu, Y.-Q. (2007). *Acta Cryst.* **E63**, m2991.
- Liu, Y., Dou, J., Li, D. & Zhang, X. (2007). *Acta Cryst.* **E63**, m2661.
- Liu, Y., He, Q., Zhang, X., Xue, Z. & Lv, C. (2008). *Acta Cryst.* **E64**, m1604.
- Liu, Y., Zhang, X., Xue, Z., He, Q. & Zhang, Y. (2008). *Acta Cryst.* **E64**, m1077.
- Lu, J. (2009). *Acta Cryst.* **E65**, m1187.
- Yang, X.-M., Leng, Q.-B., Chen, Y., He, Y.-G. & Luo, S.-W. (2009). *Acta Cryst.* **E65**, m567.
- Zhang, X., Wei, P. & Li, B. (2008). *Acta Cryst.* **E64**, m934.

## Diazidobis(2,2'-biimidazole)cobalt(II)

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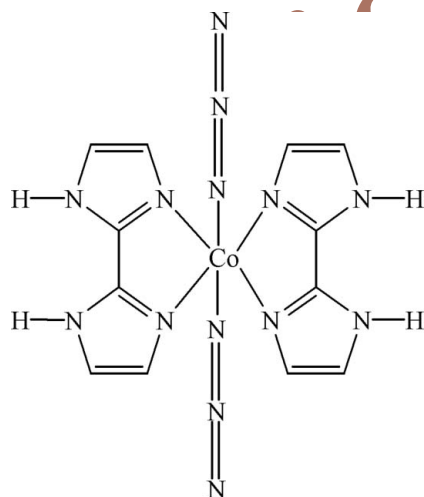
Received 10 November 2007; accepted 24 November 2007

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.078; data-to-parameter ratio = 12.1.

In the title compound,  $[\text{Co}(\text{N}_3)_2(\text{C}_6\text{H}_6\text{N}_4)_2]$ , the  $\text{Co}^{\text{II}}$  atom lies on a centre of inversion and is bonded to two azide ions and two bidentate 2,2'-biimidazole ligands, giving a slightly distorted octahedral  $\text{CoN}_6$  coordination geometry. In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds exist between the 2,2'-biimidazole ligands and the azide ions, linking the complexes into sheets.

### Related literature

For related literature, see: Rees *et al.* (1983); Hardman & Lipscomb (1984); Kuo & Makinen (1982); Dworschak & Plapp (1977).



### Experimental

#### Crystal data

$[\text{Co}(\text{N}_3)_2(\text{C}_6\text{H}_6\text{N}_4)_2]$   
 $M_r = 411.29$   
 Monoclinic,  $C2/c$   
 $a = 12.8085$  (10) Å  
 $b = 8.7632$  (5) Å  
 $c = 14.4793$  (5) Å  
 $\beta = 91.913$  (1)°

$V = 1624.30$  (17) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.09$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 $0.28 \times 0.22 \times 0.20$  mm

#### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2001)  
 $T_{\text{min}} = 0.750$ ,  $T_{\text{max}} = 0.811$

1961 measured reflections  
 1501 independent reflections  
 1246 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.078$   
 $S = 1.00$   
 1501 reflections

124 parameters  
 H atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.21$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N6}-\text{H6A}\cdots\text{N5}^{\text{i}}$	0.86	2.01	2.819 (3)	156
$\text{N7}-\text{H7A}\cdots\text{N5}^{\text{i}}$	0.86	2.25	3.012 (3)	148
$\text{N7}-\text{H7A}\cdots\text{N3}^{\text{ii}}$	0.86	2.55	3.049 (3)	118

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: BI2265).

### References

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 Kuo, L. C. & Makinen, M. W. (1982). *J. Biol. Chem.* **257**, 24–35.  
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## supporting information

*Acta Cryst.* (2008). E64, m76 [https://doi.org/10.1107/S1600536807062873]

**Diazidobis(2,2'-biimidazole)cobalt(II)****Sheng Li, Shou-Bin Wang, Fu-Li Zhang and Kun Tang****S1. Comment**

The imidazole moiety is of biochemical importance due to its presence in more than 200 metalloenzymes, such as carboxypeptidase A (CPA), carbonic anhydrase (CA), liver alcohol dehydrogenase (LADH), and superoxide dismutase (SOD) (Rees *et al.*, 1983; Hardman & Lipscomb, 1984; Kuo & Makinen, 1982; Dworschak & Plapp, 1977).

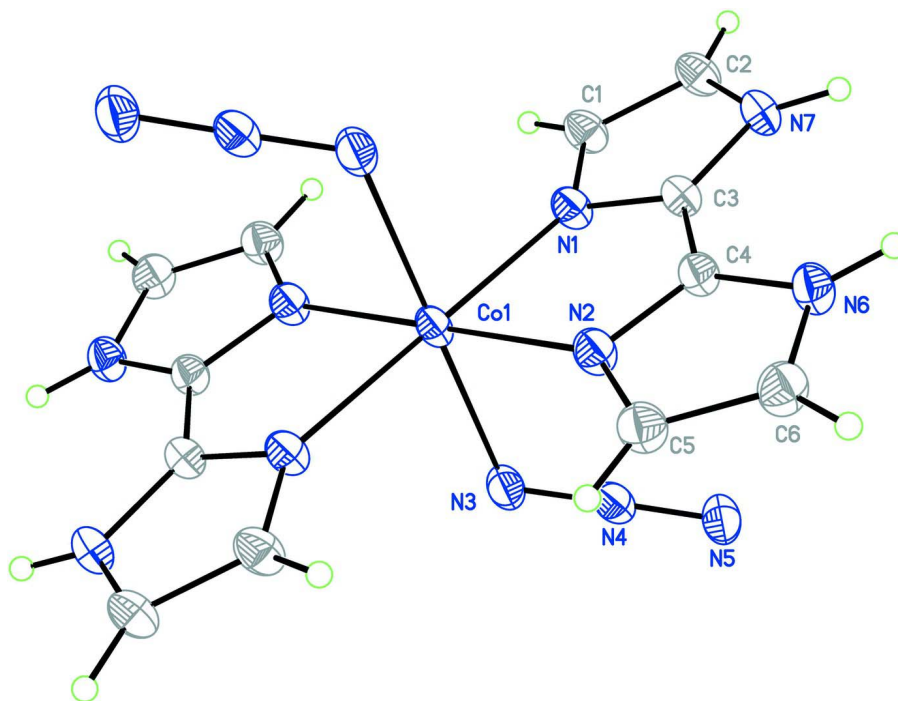
In the title compound, the Co<sup>II</sup> atom occupies an inversion centre, and is hexacoordinated by six N atoms from two chelating ligands of H<sub>2</sub>bim (2,2'-biimidazole; C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>) and two azide ions, showing a slightly distorted octahedral geometry (Fig. 1). The four N atoms from the chelating H<sub>2</sub>bim consist of the base and the other two N atoms from two azide ions occupy the axial positions. In the crystal, intermolecular N—H...N hydrogen bonds between 2,2'-biimidazole ligands and azide ions link the complexes into sheets lying in the (002) planes (Fig. 2).

**S2. Experimental**

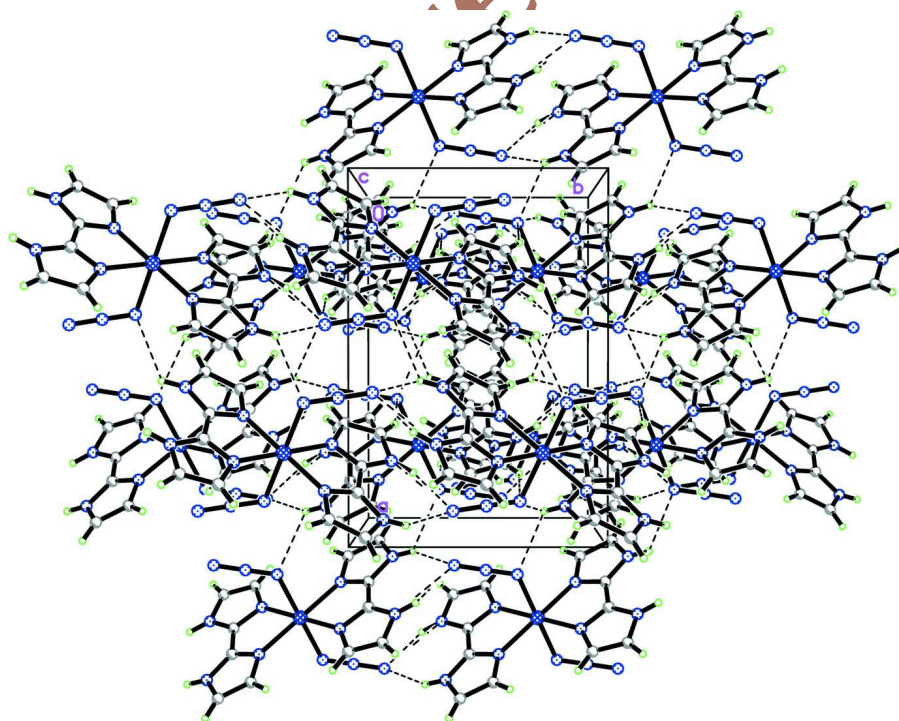
A mixture of CoCl<sub>2</sub>·2(H<sub>2</sub>O) (1 mmol), 2,2'-biimidazole (2 mmol) and NaN<sub>3</sub> (2 mmol) in 20 ml methanol was refluxed for two hours. After cooling, the solution was filtered and the filtrate was evaporated naturally at room temperature. Two days later, red blocks of the title compound were obtained with a yield of 22%. Elemental analysis calculated: C 35.04, H 2.92, N 47.69%; found: C 35.01, H 2.96, N 47.65%.

**S3. Refinement**

All H atoms were placed in calculated positions with C—H = 0.93 Å and N—H = 0.86 Å and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C/N})$ .

**Figure 1**

The molecular structure with 30% probability displacement ellipsoids for non-H atoms. Atoms with suffix I are generated by the symmetry operator  $-x + 1/2, -y - 1/2, -z + 1$ .

**Figure 2**

Packing diagram showing intermolecular N—H...N hydrogen bonds.

## Diazidobis(2,2'-biimidazole)cobalt(II)

## Crystal data

[Co(N<sub>3</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>6</sub>N<sub>4</sub>)<sub>2</sub>] $M_r = 411.29$ Monoclinic,  $C2/c$ Hall symbol:  $-C\ 2yc$  $a = 12.8085\ (10)\ \text{\AA}$  $b = 8.7632\ (5)\ \text{\AA}$  $c = 14.4793\ (5)\ \text{\AA}$  $\beta = 91.913\ (1)^\circ$  $V = 1624.30\ (17)\ \text{\AA}^3$  $Z = 4$  $F(000) = 836$  $D_x = 1.682\ \text{Mg m}^{-3}$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$ 

Cell parameters from 1501 reflections

 $\theta = 2.8\text{--}25.5^\circ$  $\mu = 1.09\ \text{mm}^{-1}$  $T = 293\ \text{K}$ 

Block, red

 $0.28 \times 0.22 \times 0.20\ \text{mm}$ 

## Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

 $T_{\min} = 0.750$ ,  $T_{\max} = 0.811$ 

1961 measured reflections

1501 independent reflections

1246 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.022$  $\theta_{\max} = 25.5^\circ$ ,  $\theta_{\min} = 2.8^\circ$  $h = -1 \rightarrow 15$  $k = -1 \rightarrow 10$  $l = -17 \rightarrow 17$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.029$  $wR(F^2) = 0.078$  $S = 1.00$ 

1501 reflections

124 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

 $w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.7528P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.016$  $\Delta\rho_{\max} = 0.24\ \text{e \AA}^{-3}$  $\Delta\rho_{\min} = -0.21\ \text{e \AA}^{-3}$ 

## 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.2500	-0.2500	0.5000	0.04053 (15)
C1	0.08433 (18)	-0.0620 (3)	0.36274 (15)	0.0523 (6)
H1	0.0724	-0.1298	0.3141	0.063*
C2	0.03681 (18)	0.0756 (3)	0.37190 (15)	0.0528 (6)

H2	-0.0126	0.1194	0.3315	0.063*
C3	0.14622 (17)	0.0371 (2)	0.48932 (14)	0.0433 (5)
C4	0.21008 (17)	0.0440 (2)	0.57427 (14)	0.0437 (5)
C5	0.32254 (19)	-0.0319 (3)	0.67815 (16)	0.0535 (6)
H5	0.3710	-0.0924	0.7103	0.064*
C6	0.29414 (19)	0.1097 (3)	0.70284 (16)	0.0556 (6)
H6	0.3182	0.1644	0.7543	0.067*
N1	0.15295 (14)	-0.0854 (2)	0.43678 (12)	0.0463 (4)
N2	0.26893 (14)	-0.0737 (2)	0.59794 (12)	0.0475 (4)
N3	0.38297 (15)	-0.1637 (2)	0.42685 (13)	0.0521 (5)
N4	0.39621 (15)	-0.0323 (2)	0.42133 (13)	0.0507 (5)
N5	0.41050 (18)	0.0987 (2)	0.41471 (16)	0.0668 (6)
N6	0.22221 (15)	0.1566 (2)	0.63634 (12)	0.0506 (5)
H6A	0.1905	0.2432	0.6348	0.061*
N7	0.07654 (14)	0.1364 (2)	0.45280 (12)	0.0484 (4)
H7A	0.0598	0.2230	0.4761	0.058*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.0437 (2)	0.0363 (2)	0.0409 (2)	0.01142 (17)	-0.00752 (16)	-0.00494 (16)
C1	0.0524 (13)	0.0580 (14)	0.0459 (12)	0.0139 (11)	-0.0072 (10)	-0.0039 (10)
C2	0.0522 (13)	0.0585 (15)	0.0473 (12)	0.0164 (11)	-0.0055 (10)	0.0043 (11)
C3	0.0431 (11)	0.0417 (12)	0.0452 (11)	0.0082 (9)	0.0015 (9)	0.0009 (9)
C4	0.0455 (11)	0.0400 (11)	0.0456 (11)	0.0047 (10)	0.0022 (9)	-0.0028 (9)
C5	0.0556 (13)	0.0536 (14)	0.0503 (12)	0.0048 (11)	-0.0100 (10)	-0.0019 (11)
C6	0.0618 (14)	0.0551 (15)	0.0491 (12)	-0.0004 (12)	-0.0088 (11)	-0.0091 (11)
N1	0.0474 (10)	0.0460 (11)	0.0450 (9)	0.0112 (9)	-0.0048 (8)	-0.0042 (8)
N2	0.0507 (10)	0.0442 (10)	0.0472 (10)	0.0078 (9)	-0.0065 (8)	-0.0044 (8)
N3	0.0554 (11)	0.0401 (11)	0.0605 (11)	0.0096 (9)	-0.0019 (9)	-0.0036 (9)
N4	0.0488 (11)	0.0505 (13)	0.0522 (11)	0.0128 (9)	-0.0073 (9)	-0.0070 (9)
N5	0.0717 (14)	0.0417 (12)	0.0860 (15)	0.0073 (11)	-0.0101 (12)	-0.0065 (11)
N6	0.0588 (11)	0.0415 (11)	0.0514 (10)	0.0074 (9)	-0.0008 (9)	-0.0070 (8)
N7	0.0531 (11)	0.0425 (10)	0.0497 (10)	0.0148 (9)	0.0018 (8)	0.0005 (8)

*Geometric parameters (Å, °)*

Co1—N1	2.0945 (17)	C3—C4	1.455 (3)
Co1—N1 <sup>i</sup>	2.0945 (17)	C4—N2	1.316 (3)
Co1—N2 <sup>i</sup>	2.1055 (18)	C4—N6	1.341 (3)
Co1—N2	2.1055 (18)	C5—C6	1.344 (3)
Co1—N3	2.172 (2)	C5—N2	1.379 (3)
Co1—N3 <sup>i</sup>	2.172 (2)	C5—H5	0.930
C1—C2	1.359 (3)	C6—N6	1.373 (3)
C1—N1	1.379 (3)	C6—H6	0.930
C1—H1	0.930	N3—N4	1.167 (3)
C2—N7	1.370 (3)	N4—N5	1.167 (3)
C2—H2	0.930	N6—H6A	0.860

C3—N1	1.320 (3)	N7—H7A	0.860
C3—N7	1.343 (3)		
N1—Co1—N1 <sup>i</sup>	180.00 (8)	N2—C4—N6	110.49 (19)
N1—Co1—N2 <sup>i</sup>	99.06 (7)	N2—C4—C3	119.23 (19)
N1 <sup>i</sup> —Co1—N2 <sup>i</sup>	80.94 (7)	N6—C4—C3	130.3 (2)
N1—Co1—N2	80.94 (7)	C6—C5—N2	109.7 (2)
N1 <sup>i</sup> —Co1—N2	99.06 (7)	C6—C5—H5	125.1
N2 <sup>i</sup> —Co1—N2	180.0	N2—C5—H5	125.1
N1—Co1—N3	90.61 (7)	C5—C6—N6	105.7 (2)
N1 <sup>i</sup> —Co1—N3	89.39 (7)	C5—C6—H6	127.1
N2 <sup>i</sup> —Co1—N3	90.10 (7)	N6—C6—H6	127.1
N2—Co1—N3	89.90 (7)	C3—N1—C1	105.96 (18)
N1—Co1—N3 <sup>i</sup>	89.39 (7)	C3—N1—Co1	110.93 (13)
N1 <sup>i</sup> —Co1—N3 <sup>i</sup>	90.61 (7)	C1—N1—Co1	142.74 (16)
N2 <sup>i</sup> —Co1—N3 <sup>i</sup>	89.90 (7)	C4—N2—C5	106.00 (19)
N2—Co1—N3 <sup>i</sup>	90.10 (7)	C4—N2—Co1	110.33 (14)
N3—Co1—N3 <sup>i</sup>	180.00 (6)	C5—N2—Co1	143.64 (16)
C2—C1—N1	109.4 (2)	N4—N3—Co1	119.70 (17)
C2—C1—H1	125.3	N5—N4—N3	179.0 (3)
N1—C1—H1	125.3	C4—N6—C6	108.01 (19)
C1—C2—N7	105.91 (19)	C4—N6—H6A	126.0
C1—C2—H2	127.0	C6—N6—H6A	126.0
N7—C2—H2	127.0	C3—N7—C2	107.90 (18)
N1—C3—N7	110.83 (19)	C3—N7—H7A	126.0
N1—C3—C4	118.37 (18)	C2—N7—H7A	126.1
N7—C3—C4	130.8 (2)		

Symmetry code: (i)  $-x+1/2, -y-1/2, -z+1$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N6—H6A $\cdots$ N5 <sup>ii</sup>	0.86	2.01	2.819 (3)	156
N7—H7A $\cdots$ N5 <sup>ii</sup>	0.86	2.25	3.012 (3)	148
N7—H7A $\cdots$ N3 <sup>iii</sup>	0.86	2.55	3.049 (3)	118

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