Acta Crystallographica Section E **Structure Reports** Online

ISSN 1600-5368

## catena-Poly[[(dipyrido[3,2-a:2',3'-c]phenazine)cobalt(II)]- $\mu$ -biphenyl-2,2'dicarboxylato]

#### Fang Wei, Wen-Ju Wang, Xiang-Jun Jin, Ze-Min Mei\* and **Xiao-Ping Li**

Department of Chemistry, Baicheng Normal College, Baicheng 137000, People's Republic of China

Correspondence e-mail: fangwei1026@yahoo.com.cn

Received 15 January 2008; accepted 17 January 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean  $\sigma$ (C–C) = 0.007 Å; R factor = 0.049; wR factor = 0.086; data-to-parameter ratio = 13.4.

In the title compound,  $[Co(C_{14}H_8O_4)(C_{18}H_{10}N_4)]_n$ , the Co<sup>II</sup> atom is six-coordinated by four O atoms from two different biphenyl-2,2'-dicarboxylate ligands and two N atoms from the bidentate dipyrido[3,2-a:2',3'-c]phenazine ligand in a distorted octahedral geometry. The Co<sup>II</sup> atoms are bridged by the biphenyl-2,2'-dicarboxylate ligands to form a one-dimensional chain structure.  $\pi$ - $\pi$  interactions between neighbouring chains result in a two-dimensional supramolecular network (centroid-to-centroid separation = 3.381 Å).

#### **Related literature**

For related literature, see: Hao et al. (2004); Li et al. (2006); Noveron et al. (2002); Dickeson & Summers (1970); Li et al. (2007); Zhang et al. (2001).

# metal-organic compounds

#### **Experimental**

#### Crystal data

$[Co(C_{14}H_8O_4)(C_{18}H_{10}N_4)]$	$V = 2486.5 (19) \text{ Å}^3$
$M_r = 581.43$	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 9.311 (4)  Å	$\mu = 0.74 \text{ mm}^{-1}$
b = 12.521 (5)  Å	T = 293 (2) K
c = 21.831 (10)  Å	$0.43 \times 0.11 \times 0.07 \text{ mm}$
$\beta = 102.31^{\circ}$	

#### Data collection

Bruker APEXII diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2002)  $T_{\min} = 0.904, \ T_{\max} = 0.951$ 

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$	370 parameters
$wR(F^2) = 0.085$	H-atom parameters constrained
S = 0.87	$\Delta \rho_{\rm max} = 0.92 \ {\rm e} \ {\rm \AA}^{-3}$
5022 reflections	$\Delta \rho_{\rm min} = -0.30 \text{ e } \text{\AA}^{-3}$

13141 measured reflections

 $R_{\rm int} = 0.085$ 

5022 independent reflections

1796 reflections with  $I > 2\sigma(I)$ 

#### Table 1

Selected geometric parameters (Å, °).

Co1-O3 <sup>i</sup>	2.087 (3)	Co1-N1	2.115 (4)
Co1-N2	2.093 (4)	Co1-O2	2.151 (3)
Co1-O1	2.105 (3)	Co1-O4 <sup>i</sup>	2.185 (3)
N2-Co1-O1	95.31 (15)	N2-Co1-O2	97.96 (13)
N2-Co1-N1	78.05 (16)	O1-Co1-O2	61.86 (10)
O1-Co1-N1	159.78 (13)	N1-Co1-O2	99.79 (13)
Symmetry code: (i) -	$r v \pm \frac{1}{2} - 7 \pm \frac{1}{2}$		

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

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL-Plus (Sheldrick, 2008); software used to prepare material for publication: SHELXTL-Plus.

The authors thank Baicheng Normal College for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2538).

#### References

- Bruker (2002). SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2006). APEX2. Bruker AXS Inc., Madison, Wisconsin, USA.

Dickeson, J. E. & Summers, L. A. (1970). Aust. J. Chem. 23, 1023-1027.

- Hao, N., Shen, E.-H., Li, Y.-G., Wang, E.-B., Hu, C.-W. & Xu, L. (2004). Inorg. Chem. Commun. 7, 510-512.
- Li, C.-B., Fang, W., Dong, E.-J., Liu, B. & Li, Y.-W. (2007). Acta Cryst. E63, m150-m152
- Li, C.-B., Fang, W., Gao, G.-G. & Liu, B. (2006). Acta Cryst. E62, m1312m1314.
- Noveron, J. C., Lah, M. S., Sesto, R. E. D., Arif, A. M., Miller, J. S. & Stang, P. J. (2002). J. Am. Chem. Soc. 124, 6613-6625.
- Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
- Zhang, H. X., Kang, B. S., Xu, A. W., Chen, Z. N., Zhou, Z. Y., Yu, K. B. & Ren, C. (2001). J. Chem. Soc. Dalton Trans. pp. 2559-2566.



## supporting information

Acta Cryst. (2008). E64, m379 [doi:10.1107/S1600536808001827]

## *catena*-Poly[[(dipyrido[3,2-*a*:2',3'-*c*]phenazine)cobalt(II)]-μ-biphenyl-2,2'-dicarboxylato]

## Fang Wei, Wen-Ju Wang, Xiang-Jun Jin, Ze-Min Mei and Xiao-Ping Li

### S1. Comment

Metal-organic hybrid compounds have attracted considerable interest and importance in recent years, not only due to their intriguing structural motifs but also their potential applications in areas such as catalysis, medicine and host–guest chemistry (Hao *et al.*, 2004). The chelating ligand 1,10-phenanthroline (phen) and its derivatives have been widely used in the construction of metal-organic coordination polymers (Li *et al.*, 2006). On the other hand, carboxylate ligands have already been proven to be efficient for the generation of a helical coordination polymer (Li *et al.*, 2007), so we reacted dipydo[3,2 - a:2',3'-c]phenazine with cobalt and biphenyl-2,2'-dicarboxylate, resulting in the title molecular complex,  $[Co(C_{14}H_8O_4)(C_{18}H_{10}N_4)]_n$ , (I)

Compound (I) is a one-dimensional chain structure, which is constructed from one  $Co^{II}$  atom, one *L* ligand and two biphenyl-2,2'-dicarboxylate dianion (Fig. 1). The  $Co^{II}$  center is six-coordinated by two N atoms from the bidentate *L* ligand and four O atoms from two different 2,6'-biphenyl dicarboxylic acid ligands to result in a substantially distorted *cis*- $CoN_2O_4$  octahedron. The mean Co—O and Co—N distances are 2.112 (3) and 2.104 (4) Å, respectively. The C—O bond lengths of the 2,6'-biphenyl dicarboxylic acid groups imply electronic delocalizations of the negative charges.

Neighboring Co<sup>II</sup> atoms are bridged by the biphenyl-2,2'-dicarboxylate ligands, forming a one-dimensional chain structure as shown in (Fig. 2). Then, neighbouring chains are connected by  $\pi$ - $\pi$  interactions, generating a two-dimensional supramolecular structure (Fig. 3). The  $\pi$ - $\pi$  stacking distances are 3.381Å between *L* ligands. Similar values are seen in related structures (Noveron *et al.*, 2002).

#### **S2. Experimental**

The *L* ligand was synthesized by the literature method of Dickeson & Summers (1970). A mixture of  $CoCl_2.2H_2O$  (0.3 mmol), *L* (0.1 mmol) and 2,6'-biphenyl dicarboxylic acid (0.3 mmol) in 30 ml of distilled water was stirred thoroughly for 1 h at ambient temperature. The pH value was adjusted to about 7.5 with NaOH aqueous solution. The suspension was sealed in a Teflon-lined stainless reaction vessel (40 ml) and heated at 443 K for 5 days. The vessel was cooled slowly to room temperature at a rate of 10 K h<sup>-1</sup> before opening and yellow crystals of (I) were collected.

#### S3. Refinement

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



### Figure 1

The asymmetric unit of (I), together with additional atoms to complete the coordination of Co1 with displacement ellipsoids drawn at the 30% probability level (arbitrary spheres for the H atoms). Symmetry codes: (i) -x, -y + 1/2, -z + 1/2; (ii) -x, y - 1/2, -z + 1/2.



### Figure 2

A view of the one-chain structure of (I). H atoms have been omitted for clarity.



#### Figure 3

View of the two-dimensional supramolecular structure of (I) generated by  $\pi$ - $\pi$  interations. H atoms have been omitted for clarity.

F(000) = 1188.0 $D_{\rm x} = 1.553 \text{ Mg m}^{-3}$ 

 $\theta = 2.3-26.0^{\circ}$   $\mu = 0.74 \text{ mm}^{-1}$  T = 293 KBlock, amethyst  $0.44 \times 0.11 \times 0.07 \text{ mm}$ 

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å Cell parameters from 2096 reflections

#### catena-Poly[[(dipyrido[3,2 - a:2',3'-c]phenazine)cobalt(II)]-µ-biphenyl-2,2'- dicarboxylato]

Crystal data
$[Co(C_{14}H_8O_4)(C_{18}H_{10}N_4)]$
$M_r = 581.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 9.311 (4)  Å
b = 12.521 (5)  Å
c = 21.831 (10)  Å
$\beta = 102.31^{\circ}$
$V = 2486.5 (19) \text{ Å}^3$
Z = 4
Data collection

Bruker APEXII	13141 measured reflections
diffractometer	5022 independent reflections
Radiation source: fine-focus sealed tube	1796 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\rm int} = 0.085$
Detector resolution: 0 pixels mm <sup>-1</sup>	$\theta_{\text{max}} = 26.2^{\circ}, \ \theta_{\text{min}} = 1.9^{\circ}$
not measured scans	$h = -9 \rightarrow 11$
Absorption correction: multi-scan	$k = -15 \rightarrow 15$
(SADABS; Bruker, 2002)	$l = -27 \rightarrow 18$
$T_{\min} = 0.904, \ T_{\max} = 0.951$	

Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier
Least-squares matrix: full	map
$R[F^2 > 2\sigma(F^2)] = 0.048$	Hydrogen site location: inferred from
$wR(F^2) = 0.085$	neighbouring sites
S = 0.87	H-atom parameters constrained
5022 reflections	$w = 1/[\sigma^2(F_o^2) + (0.002P)^2]$
370 parameters	where $P = (F_{o}^{2} + 2F_{c}^{2})/3$
0 restraints	$(\Delta/\sigma)_{\rm max} = 0.001$
Primary atom site location: structure-invariant	$\Delta  ho_{ m max} = 0.92 \ { m e} \ { m \AA}^{-3}$
direct methods	$\Delta \rho_{\min} = -0.30 \text{ e} \text{ Å}^{-3}$

#### 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  $(A^2)$ 

	x	У	Ζ	$U_{ m iso}$ */ $U_{ m eq}$
Col	0.02037 (7)	0.27680 (5)	0.19183 (3)	0.0511 (2)
01	0.1414 (3)	0.2191 (3)	0.27808 (13)	0.0644 (10)
O2	-0.0977 (3)	0.2343 (2)	0.26292 (13)	0.0526 (9)
N2	0.0064 (4)	0.1293 (3)	0.14589 (18)	0.0486 (11)
C5	-0.3420 (5)	0.1185 (4)	-0.0118 (2)	0.0458 (13)
N1	-0.1583 (4)	0.3017 (3)	0.11521 (17)	0.0496 (11)
C4	-0.3106 (5)	0.2151 (4)	0.0256 (2)	0.0455 (13)
C12	-0.2475 (5)	0.0282 (4)	0.0016 (2)	0.0449 (13)
N4	-0.4625 (4)	0.1169 (3)	-0.05836 (18)	0.0521 (12)
C13	-0.1245 (5)	0.0309 (4)	0.0561 (2)	0.0454 (13)
N3	-0.2692 (4)	-0.0605 (3)	-0.03208 (19)	0.0512 (11)
C18	-0.1927 (5)	0.2156 (4)	0.0769 (2)	0.0436 (12)
C17	-0.1001 (5)	0.1222 (4)	0.0925 (2)	0.0422 (13)
C19	0.0254 (5)	0.2107 (4)	0.2984 (2)	0.0457 (13)
C6	-0.4883 (5)	0.0253 (5)	-0.0920 (2)	0.0519 (14)
C20	0.0350 (5)	0.1783 (3)	0.3653 (2)	0.0395 (12)
C31	-0.2806 (5)	0.0171 (4)	0.3290 (2)	0.0454 (13)
C26	-0.2356 (5)	0.1185 (4)	0.3516 (2)	0.0461 (13)
C11	-0.3907 (6)	-0.0624 (4)	-0.0800(2)	0.0526 (14)
C23	0.0737 (5)	0.1393 (4)	0.4925 (2)	0.0661 (16)
H23A	0.0846	0.1279	0.5354	0.079*
C21	0.1700 (5)	0.1932 (3)	0.4056 (2)	0.0498 (14)
H21A	0.2490	0.2170	0.3894	0.060*
C3	-0.3955 (5)	0.3080 (4)	0.0141 (2)	0.0569 (15)
H3B	-0.4744	0.3108	-0.0201	0.068*

C25	-0.0827 (5)	0.1402 (4)	0.3883 (2)	0.0454 (13)
C24	-0.0610 (5)	0.1215 (4)	0.4522 (2)	0.0587 (15)
H24A	-0.1390	0.0963	0.4686	0.070*
C30	-0.4302 (6)	-0.0057 (4)	0.3079 (2)	0.0628 (16)
H30A	-0.4597	-0.0743	0.2944	0.075*
C7	-0.6179 (5)	0.0173 (4)	-0.1408 (2)	0.0602 (16)
H7A	-0.6833	0.0743	-0.1490	0.072*
C14	-0.0337 (5)	-0.0574 (4)	0.0756 (2)	0.0569 (15)
H14A	-0.0458	-0.1199	0.0520	0.068*
C27	-0.3441 (6)	0.1970 (4)	0.3493 (2)	0.0624 (15)
H27A	-0.3163	0.2656	0.3634	0.075*
C2	-0.3632 (5)	0.3954 (4)	0.0528 (2)	0.0692 (17)
H2B	-0.4201	0.4570	0.0460	0.083*
C16	0.0876 (5)	0.0434 (5)	0.1629 (2)	0.0578 (15)
H16A	0.1594	0.0471	0.1997	0.069*
C1	-0.2411 (5)	0.3880 (4)	0.1032 (2)	0.0574 (15)
H1B	-0.2174	0.4469	0.1294	0.069*
C10	-0.4203 (6)	-0.1538 (4)	-0.1182 (3)	0.0649 (16)
H10A	-0.3551	-0.2110	-0.1123	0.078*
C15	0.0737 (5)	-0.0517 (4)	0.1299 (3)	0.0635 (16)
H15A	0.1344	-0.1097	0.1438	0.076*
C22	0.1907 (5)	0.1739 (4)	0.4688 (2)	0.0571 (15)
H22A	0.2823	0.1840	0.4951	0.069*
C29	-0.5345 (6)	0.0734 (5)	0.3071 (2)	0.0678 (16)
H29A	-0.6337	0.0578	0.2932	0.081*
C28	-0.4916 (6)	0.1750 (5)	0.3267 (2)	0.0697 (17)
H28A	-0.5613	0.2287	0.3248	0.084*
C8	-0.6444 (6)	-0.0731 (5)	-0.1747 (2)	0.0716 (18)
H8A	-0.7299	-0.0790	-0.2055	0.086*
C9	-0.5458 (7)	-0.1579 (5)	-0.1642 (2)	0.0695 (17)
H9A	-0.5655	-0.2188	-0.1890	0.083*
C32	-0.1725 (6)	-0.0692 (4)	0.3244 (2)	0.0483 (14)
O3	-0.1965 (3)	-0.1613 (3)	0.34207 (15)	0.0616 (10)
O4	-0.0650 (3)	-0.0519 (2)	0.30026 (15)	0.0594 (10)

Atomic displacement parameters  $(\mathring{A}^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Col	0.0506 (4)	0.0622 (5)	0.0386 (4)	-0.0010 (4)	0.0055 (3)	0.0012 (4)
01	0.0366 (19)	0.114 (3)	0.044 (2)	0.004 (2)	0.0134 (17)	0.015 (2)
02	0.0424 (19)	0.076 (2)	0.038 (2)	0.0024 (18)	0.0062 (16)	0.0077 (18)
N2	0.050 (3)	0.051 (3)	0.043 (3)	0.000 (2)	0.004 (2)	0.005 (2)
C5	0.039 (3)	0.064 (4)	0.036 (3)	-0.006 (3)	0.013 (3)	0.007 (3)
N1	0.048 (3)	0.059 (3)	0.040 (3)	0.005 (2)	0.006 (2)	0.000(2)
C4	0.036 (3)	0.060 (4)	0.040 (3)	-0.003 (3)	0.006 (2)	0.002 (3)
C12	0.043 (3)	0.056 (4)	0.038 (3)	-0.008 (3)	0.013 (3)	0.004 (3)
N4	0.046 (3)	0.072 (3)	0.039 (3)	-0.008(2)	0.009 (2)	0.001 (2)
C13	0.042 (3)	0.054 (4)	0.042 (3)	-0.003 (3)	0.014 (3)	0.006 (3)

## supporting information

N3	0.051 (3)	0.060 (3)	0.045 (3)	-0.013 (2)	0.015 (2)	-0.006 (2)
C18	0.040 (3)	0.056 (4)	0.036 (3)	-0.005 (3)	0.012 (2)	0.001 (3)
C17	0.039 (3)	0.051 (4)	0.039 (3)	-0.005 (3)	0.014 (3)	0.007 (3)
C19	0.047 (3)	0.046 (3)	0.043 (3)	-0.002 (3)	0.007 (3)	-0.005 (3)
C6	0.051 (4)	0.066 (4)	0.040 (4)	-0.015 (3)	0.014 (3)	-0.002 (3)
C20	0.038 (3)	0.047 (3)	0.031 (3)	0.001 (3)	0.001 (2)	0.000(2)
C31	0.039 (3)	0.062 (4)	0.035 (3)	-0.001 (3)	0.008 (3)	0.002 (3)
C26	0.039 (3)	0.066 (4)	0.037 (3)	0.003 (3)	0.014 (3)	0.009 (3)
C11	0.060 (4)	0.063 (4)	0.041 (4)	-0.022 (3)	0.025 (3)	-0.004 (3)
C23	0.063 (4)	0.097 (5)	0.035 (3)	0.011 (4)	0.003 (3)	0.007 (3)
C21	0.049 (3)	0.060 (4)	0.041 (3)	-0.003 (3)	0.012 (3)	-0.005 (3)
C3	0.042 (3)	0.072 (4)	0.052 (4)	0.004 (3)	0.001 (3)	0.004 (3)
C25	0.040 (3)	0.055 (3)	0.041 (3)	0.003 (3)	0.005 (3)	0.001 (3)
C24	0.049 (3)	0.084 (4)	0.043 (4)	-0.005 (3)	0.011 (3)	0.004 (3)
C30	0.056 (4)	0.076 (4)	0.056 (4)	-0.003 (3)	0.010 (3)	0.004 (3)
C7	0.052 (4)	0.084 (5)	0.043 (4)	-0.016 (3)	0.009 (3)	0.004 (3)
C14	0.053 (3)	0.062 (4)	0.060 (4)	-0.010 (3)	0.022 (3)	-0.002 (3)
C27	0.053 (4)	0.069 (4)	0.067 (4)	0.003 (3)	0.018 (3)	0.002 (3)
C2	0.066 (4)	0.069 (4)	0.065 (4)	-0.002 (3)	-0.003 (3)	-0.011 (4)
C16	0.051 (3)	0.072 (4)	0.048 (4)	0.005 (3)	0.007 (3)	0.008 (4)
C1	0.058 (4)	0.057 (4)	0.055 (4)	0.011 (3)	0.009 (3)	-0.014 (3)
C10	0.076 (4)	0.068 (4)	0.058 (4)	-0.015 (3)	0.029 (3)	-0.010 (3)
C15	0.062 (4)	0.061 (4)	0.068 (4)	0.001 (3)	0.016 (3)	0.001 (4)
C22	0.047 (3)	0.074 (4)	0.046 (4)	0.002 (3)	-0.001 (3)	-0.002 (3)
C29	0.037 (3)	0.103 (5)	0.062 (4)	-0.004 (4)	0.006 (3)	0.006 (4)
C28	0.048 (4)	0.091 (5)	0.073 (4)	0.011 (4)	0.019 (3)	0.007 (4)
C8	0.074 (5)	0.097 (5)	0.044 (4)	-0.028 (4)	0.011 (3)	0.004 (4)
C9	0.090 (5)	0.079 (5)	0.042 (4)	-0.034 (4)	0.019 (4)	-0.016 (3)
C32	0.052 (4)	0.056 (4)	0.032 (3)	-0.001 (4)	-0.002 (3)	-0.007 (3)
O3	0.066 (2)	0.057 (2)	0.070 (3)	0.004 (2)	0.032 (2)	0.006 (2)
O4	0.050 (2)	0.068 (3)	0.063 (2)	0.003 (2)	0.019 (2)	0.004 (2)

## Geometric parameters (Å, °)

Co1–O3 <sup>i</sup>	2.087 (3)	C23—C22	1.372 (5)
Co1—N2	2.093 (4)	C23—C24	1.388 (5)
Co101	2.105 (3)	C23—H23A	0.9300
Co1—N1	2.115 (4)	C21—C22	1.374 (5)
Co1—O2	2.151 (3)	C21—H21A	0.9300
Co1—O4 <sup>i</sup>	2.185 (3)	C3—C2	1.376 (5)
Co1-C19	2.460 (5)	С3—Н3В	0.9300
Co1-C32 <sup>i</sup>	2.463 (6)	C25—C24	1.386 (5)
O1—C19	1.256 (4)	C24—H24A	0.9300
O2—C19	1.274 (4)	C30—C29	1.384 (6)
N2—C16	1.322 (5)	C30—H30A	0.9300
N2—C17	1.363 (5)	C7—C8	1.346 (6)
C5—N4	1.344 (5)	С7—Н7А	0.9300
C5—C12	1.424 (6)	C14—C15	1.381 (6)

C5—C4	1.454 (6)	C14—H14A	0.9300
N1—C1	1.322 (5)	C27—C28	1.384 (6)
N1—C18	1.360 (5)	С27—Н27А	0.9300
C4—C18	1.391 (5)	C2—C1	1.406 (5)
C4—C3	1.398 (5)	C2—H2B	0.9300
C12—N3	1.323 (5)	C16—C15	1.383 (5)
C12—C13	1.465 (5)	C16—H16A	0.9300
N4—C6	1.355 (5)	C1—H1B	0.9300
C13—C17	1.384 (6)	С10—С9	1.369 (6)
C13—C14	1.402 (6)	C10—H10A	0.9300
N3—C11	1.367 (5)	C15—H15A	0.9300
C18—C17	1.450 (6)	C22—H22A	0.9300
C19—C20	1.501 (6)	C29—C28	1.374 (6)
C6—C11	1.414 (6)	С29—Н29А	0.9300
С6—С7	1.432 (6)	C28—H28A	0.9300
C20—C25	1.384 (5)	C8—C9	1.390 (6)
C20—C21	1.385 (5)	C8—H8A	0.9300
C31—C26	1.394 (6)	С9—Н9А	0.9300
C31—C30	1.400 (5)	C32—O4	1.246 (5)
C31—C32	1,494 (6)	C32—O3	1.252 (5)
C26—C27	1.403 (5)	C32—Co1 <sup>ii</sup>	2.463 (6)
C26—C25	1.502 (5)	O3—Co1 <sup>ii</sup>	2.087 (3)
C11—C10	1.409 (6)	O4—Co1 <sup>ii</sup>	2.185 (3)
			()
O3 <sup>i</sup> —Co1—N2	97.50 (14)	C31—C26—C27	117.8 (5)
O3 <sup>i</sup> —Co1—O1	97.66 (12)	C31—C26—C25	122.2 (5)
N2—Co1—O1	95.31 (15)	C27—C26—C25	119.0 (5)
O3 <sup>i</sup> —Co1—N1	102.12 (13)	N3—C11—C10	119.5 (6)
N2—Co1—N1	78.05 (16)	N3—C11—C6	121.5 (5)
O1—Co1—N1	159.78 (13)	C10—C11—C6	119.0 (5)
O3 <sup>i</sup> —Co1—O2	155.35 (12)	C22—C23—C24	119.6 (5)
N2—Co1—O2	97.96 (13)	С22—С23—Н23А	120.2
O1—Co1—O2	61.86 (10)	C24—C23—H23A	120.2
N1—Co1—O2	99.79 (13)	C22—C21—C20	121.8 (5)
O3 <sup>i</sup> —Co1—O4 <sup>i</sup>	60.87 (12)	C22—C21—H21A	119.1
N2—Co1—O4 <sup>i</sup>	153.61 (14)	C20—C21—H21A	119.1
O1—Co1—O4 <sup>i</sup>	102.11 (12)	C2—C3—C4	120.6 (5)
N1—Co1—O4 <sup>i</sup>	91.27 (14)	С2—С3—Н3В	119.7
O2—Co1—O4 <sup>i</sup>	107.67 (12)	C4—C3—H3B	119.7
O3 <sup>i</sup> —Co1—C19	127.04 (14)	C20—C25—C24	117.8 (4)
N2—Co1—C19	98.21 (15)	C20—C25—C26	127.0 (4)
O1—Co1—C19	30.71 (11)	C24—C25—C26	115.1 (4)
N1—Co1—C19	130.56 (15)	C25—C24—C23	121.9 (5)
O2—Co1—C19	31.16 (11)	C25—C24—H24A	119.0
$O4^{i}$ —Co1—C19	106.91 (14)	C23—C24—H24A	119.0
$O3^{i}$ — $C01$ — $C32^{i}$	30.54 (13)	$C_{29}$ $C_{30}$ $C_{31}$	120.3 (5)
$N2-Co1-C32^{i}$	126.93 (16)	C29—C30—H30A	119.9
			110.0

N1-Co1-C32 <sup>i</sup>	98.65 (15)	C8—C7—C6	119.6 (5)
$02-Co1-C32^{i}$	134.08 (15)	C8—C7—H7A	120.2
$O4^{i}$ —Co1—C32 <sup>i</sup>	30.36 (12)	С6—С7—Н7А	120.2
C19—Co1—C32 <sup>i</sup>	120.29 (15)	C15—C14—C13	120.0 (5)
C19—O1—Co1	90.5 (3)	C15—C14—H14A	120.0
C19—O2—Co1	87.9 (3)	C13—C14—H14A	120.0
C16 - N2 - C17	117.1 (4)	C28—C27—C26	121.7 (5)
C16—N2—Co1	127.6 (4)	С28—С27—Н27А	119.2
C17 - N2 - Co1	115.3 (3)	С26—С27—Н27А	119.2
N4—C5—C12	121.5 (5)	$C_3 - C_2 - C_1$	117.6 (5)
N4—C5—C4	118.2 (5)	C3—C2—H2B	121.2
C12—C5—C4	120.3(5)	C1-C2-H2B	121.2
C1-N1-C18	1184(4)	$N_{-C16-C15}$	124.8 (5)
C1-N1-Co1	127 2 (4)	N2-C16-H16A	117.6
C18 - N1 - Co1	1143(3)	$C_{15}$ $C_{16}$ $H_{16A}$	117.6
C18 - C4 - C3	117.4 (5)	N1-C1-C2	123 3 (5)
C18 - C4 - C5	117.4(5) 119.0(5)	N1—C1—H1B	118.3
$C_{3}$ $C_{4}$ $C_{5}$	123.5(4)	$C_2 - C_1 - H_1B$	118.3
$N_{3}$ $C_{12}$ $C_{5}$	122.5 (4)	$C_{2} = C_{10} = C_{11}$	119.5 (5)
$N_{3}$ $C_{12}$ $C_{3}$	122.3(5) 1181(5)	C9-C10-H10A	120.2
$C_{5}$ $C_{12}$ $C_{13}$	119 3 (5)	$C_{11}$ $C_{10}$ $H_{10A}$	120.2
$C_{5}$ N4-C6	116.5 (4)	$C_{14}$ $C_{15}$ $C_{16}$	120.2 117.5(5)
C17 - C13 - C14	117.5 (5)	$C_{14} = C_{15} = H_{15A}$	121.2
C17 - C13 - C14	117.3 (5)	$C_{16}$ $C_{15}$ $H_{15A}$	121.2
C14 - C13 - C12	117.5(5) 123.0(5)	$C_{23}$ $C_{22}$ $C_{21}$	121.2 1189(4)
C12 = N3 = C12	125.0(5) 116.3(4)	$C_{23} = C_{22} = C_{21}$	120.6
N1 - C18 - C4	122.7(5)	$C_{23} = C_{22} = H_{22} A$	120.0
N1  C18  C17	122.7(3) 116.4(4)	$C_{21} = C_{22} = \Pi_{22} R$	120.0
C4-C18-C17	120.9 (5)	$C_{28} = C_{29} = C_{30}$	110.0
$N_{2}$ $C_{17}$ $C_{13}$	120.9(5)	$C_{20} = C_{20} = H_{20} A$	119.9
$N_2 = C_{17} = C_{15}$	125.1(5) 115.0(5)	$C_{20} = C_{29} = M_{29} = M_{29}$	119.9
12 - 17 - 18	113.9(5)	$C_{29} = C_{28} = C_{27}$	119.7 (5)
01  02	121.0(3) 1107(4)	$C_{23} = C_{23} = H_{28A}$	120.1
01 - 019 - 02	119.7 (4)	$C_{2}^{7} - C_{2}^{8} - C_{2}^{9}$	120.1
01 - 019 - 020	119.3(4) 120.0(4)	C7 C8 H8A	121.0 (0)
02 - 019 - 020	120.9(4)	$C_{1} = C_{2} = H_{2}$	119.5
$0^{2}$ $C^{19}$ $C^{11}$	50.0(2)	$C_{2} = C_{3} = M_{3} \times K_{3}$	119.5
$C_{2}^{}$	175 A (2)	$C_{10} = C_{9} = C_{8}$	121.3(0)
$C_{20}$ $C_{19}$ $C_{01}$	1/3.4(3)	$C_{10}$ $C_{20}$ $H_{0A}$	119.2
N4 = C6 = C7	121.0(5)	$C_{0}$ $C_{2}$ $C_{3}$ $C_{3}$	119.2
N4-C0-C7	119.1(3) 110.2(5)	04 - 032 - 03	120.2(3)
C11 - C0 - C7	119.5 (3)	04 - 032 - 031	121.1(3)
$C_{23} = C_{20} = C_{21}$	119.9 (4)	03 - 03 - 031	110.0(3)
$C_{23} = C_{20} = C_{19}$	124.0 (4)	$0^{-1}$ $0^{-1}$ $0^{-1}$	02.4 (3) 57.0 (2)
$C_2 = C_2 $	110.0 (4)	$03 - 032 - 001^{\circ}$	3/.9(3)
C20-C31-C30	120.3 (5)	C31—C32—C01"	1/2.7 (3)

C26—C31—C32	121.8 (5)	C32—O3—Co1 <sup>ii</sup>	91.6 (3)
C30—C31—C32	117.9 (5)	C32—O4—Co1 <sup>ii</sup>	87.3 (3)

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