V = 1866.3 (7) Å³

Mo $K\alpha$ radiation $\mu = 0.53 \text{ mm}^{-1}$

 $0.40 \times 0.30 \times 0.10 \text{ mm}$

9499 measured reflections

3635 independent reflections

2640 reflections with $I > 2\sigma(I)$

H atoms treated by a mixture of

independent and constrained

Z = 2

T = 293 K

 $R_{\rm int} = 0.041$

refinement $\Delta \rho_{\text{max}} = 0.71 \text{ e } \text{\AA}^{-3}$

 $\Delta \rho_{\rm min} = -0.36 \text{ e } \text{\AA}^{-3}$

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Diaquabis[1,2-bis(pyridin-4-yl)ethene]bis[2-(4-carboxyphenyl)acetato]cobalt(II)

Wei-Hua Yu, Jian-Lan Liu and Xiao-Ming Ren*

College of Science, Nanjing University of Technology, Nanjing 210009, People's Republic of China

Correspondence e-mail: duanhaibao4660@163.com

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.105; data-to-parameter ratio = 13.6.

The asymmetric unit of the title compound, $[Co(C_9H_7O_4)_2 (C_{12}H_{10}N_2)_2(H_2O)_2]$, consists of one Co^{2+} ion, one monodeprotonated 2-(4-carboxylatophenyl)acetate carboxylic acid, one 1,2-bis(pyridin-4-yl)ethane molecule and one water molecule. The Co^{II} atom is situated on a crystallographic center of inversion and is octahedrally coordinated by two O atoms from two anions, two N atoms of two 1,2-bis(pyridin-4-yl)ethane molecules and two O atoms from two water molecules. A three-dimensional network is established by intermolecular $O-H\cdots O$ and $O-H\cdots N$ hydrogen bonds.

Related literature

For general background to the design of metal-organic supramolecular solids with potential functionality, see: Moulton & Zaworotko (2001); Janiak (2003). For weak non-covalent interactions in supramolecular solids, see: Hosseini (2005); Nishio (2004). For metal-organic supramolecular frameworks based on organic connectors containing pyridyl and/or carboxylate groups, see: Brammer (2004).



Experimental

Crystal data

 $\begin{bmatrix} Co(C_9H_7O_4)_2(C_{12}H_{10}N_2)_2(H_2O)_2 \end{bmatrix}$ $M_r = 817.69$ Monoclinic, $P2_1/c$ a = 21.349 (5) Å b = 5.6522 (12) Å c = 15.659 (4) Å $\beta = 98.999$ (4)°

Data collection

Bruker SMART CCD area-detector diffractometer Absorption correction: multi-scan (SADABS; Bruker, 2000) $T_{\rm min} = 0.850, T_{\rm max} = 0.874$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.055$ $wR(F^2) = 0.105$ S = 1.063635 reflections 268 parameters

 Table 1

 Hydrogen-bond geometry (Å, °).

2.13 (4)	2 822 (3)	158 (4)
	2.022 (3)	130 (4)
1.74 (4)	2.610 (3)	145 (3)
1.85	2.667 (3)	173
	1.74(4) 1.85	$\begin{array}{ccc} 1.74 (4) & 2.610 (3) \\ 1.85 & 2.667 (3) \\ \hline -r & -v + 1 & -z' (ijj) & -r + 1 & v - z' \\ \end{array}$

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: IM2300).

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Diaquabis[1,2-bis(pyridin-4-yl)ethene]bis[2-(4-carboxyphenyl)acetato]cobalt(II)

W.-H. Yu, J.-L. Liu and X.-M. Ren

Comment

During the past decade, the design of new metal-organic supramolecular solids has attracted ever-increasing focus in the fields of coordination chemistry and crystal engineering, for the sake of developing desired crystalline materials with potential functionality (Moulton & Zaworotko, 2001; Janiak *et al.*, 2003). Furthermore, it has been realised that weak noncovalent interactions such as hydrogen bonds, aromatic stacking, and van der Waals forces (Hosseini, 2005; Nishio, 2004) are crucial in the direction of such crystalline architectures. Hitherto, a variety of organic connectors containing pyridyl and/or carboxylate groups (Brammer, 2004) have been widely used to construct metal-organic supramolecular frameworks. Herein we report the crystal structure of the title compound (1).

The molecular structure of (1) is illustrated in Fig. 1. Compound (1) crystallizes in the monoclinic space group $P2_1/c$.

The structure of (1) is a single molecule, in which the Co^{2+} center is situated on a crystallographic center of inversion. The coordination sphere of cobalt is a slightly distorted octahedron and consistes of by two O atoms from two mono-deprotonated (4-carboxyphenyl)acetate groups, two N atoms of two 1,2-di(pyridin-4-yl)ethane molecules and two O atoms from two water molecules. As shown in Fig. 2, a one-dimensional chain is formed by O–H…N hydrogen bonds. In addition, these one-dimensional chains are linked together by additional O–H…O hydrogen bonds between water molecules and the cobalt bound carboxylate group generating a three-dimensional framework.

Experimental

Cobalt chloride hexahydrate (1 mmol), 1,2-di(pyridin-4-yl)ethane (1 mmol) and (4-carboxyphenyl)acetic acid (1 mmol) in water (8 ml) were placed in a Teflon-lined stainless-steel Parr bomb that was heated to 433 K for 48 h. Red plate crystals were collected after the bomb was subsequently allowed to cool to room temperature (yield: 38%).

Refinement

C-bound H atoms were placed geometrically (C—H = 0.93, and 0.98 Å) and refined as riding atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. O-bound H atoms were located in difference Fourier maps and refined as riding in their as-found relative positions (O—H =0.96 Å) with $U_{iso}(H) = 1.5U_{eq}(C)$.

Figures



Fig. 1. Molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

Fig. 2. One-dimensional chain structure of (I).

Diaquabis[1,2-bis(pyridin-4-yl)ethene]bis[2-(4- carboxylphenyl)acetato]cobalt(II)

Crystal data	
$[Co(C_9H_7O_4)_2(C_{12}H_{10}N_2)_2(H_2O)_2]$	F(000) = 850
$M_r = 817.69$	$D_{\rm x} = 1.455 {\rm ~Mg~m}^{-3}$
Monoclinic, $P2_1/c$	Mo K α radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 870 reflections
a = 21.349 (5) Å	$\theta = 2.6 - 22.1^{\circ}$
b = 5.6522 (12) Å	$\mu = 0.53 \text{ mm}^{-1}$
c = 15.659 (4) Å	T = 293 K
$\beta = 98.999 \ (4)^{\circ}$	Plate, red
V = 1866.3 (7) Å ³	$0.40 \times 0.30 \times 0.10 \text{ mm}$
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	3635 independent reflections
Radiation source: fine-focus sealed tube	2640 reflections with $I > 2\sigma(I)$
graphite	$R_{\rm int} = 0.041$
ϕ and ω scans	$\theta_{\text{max}} = 26.0^{\circ}, \ \theta_{\text{min}} = 1.9^{\circ}$
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 2000)	$h = -26 \rightarrow 23$
$T_{\min} = 0.850, T_{\max} = 0.874$	$k = -6 \rightarrow 6$
9499 measured reflections	$l = -19 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.055$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.105$	H atoms treated by a mixture of independent and constrained refinement
<i>S</i> = 1.06	$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.440P]$ where $P = (F_o^2 + 2F_c^2)/3$
3635 reflections	$(\Delta/\sigma)_{max} < 0.001$
268 parameters	$\Delta \rho_{max} = 0.71 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta \rho_{\rm min} = -0.36 \text{ e } \text{\AA}^{-3}$

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 coord	inates and isotropic o	or equivalent isotrop	<i>ic displacement</i>	parameters ($(Å^2)$)

	x	У	Ζ	Uiso*/Ueq
C1	0.13939 (13)	0.6024 (5)	0.07330 (17)	0.0285 (6)
H1	0.1308	0.7388	0.0404	0.034*
C2	0.21300 (13)	0.3771 (6)	0.16945 (19)	0.0324 (7)
C3	0.16536 (14)	0.2132 (6)	0.1675 (2)	0.0418 (8)
НЗА	0.1727	0.0750	0.1997	0.050*
C4	0.19847 (13)	0.5792 (5)	0.11978 (18)	0.0305 (7)
H4	0.2287	0.6969	0.1183	0.037*
C5	0.10794 (14)	0.2501 (5)	0.11927 (19)	0.0360 (7)
H5A	0.0771	0.1338	0.1194	0.043*
C6	0.27478 (13)	0.3325 (6)	0.2271 (2)	0.0446 (8)
Н6	0.2805	0.2017	0.2635	0.053*
C7	0.32607 (15)	0.5046 (7)	0.2236 (2)	0.0542 (9)
H7	0.3213	0.6348	0.1868	0.065*
C8	0.38736 (14)	0.4545 (6)	0.2844 (2)	0.0435 (8)
C9	0.43624 (15)	0.6125 (7)	0.2885 (2)	0.0480 (9)
Н9	0.4317	0.7491	0.2549	0.058*
C10	0.49294 (15)	0.5670 (6)	0.3433 (2)	0.0418 (8)
H10	0.5263	0.6730	0.3439	0.050*
C11	0.45391 (15)	0.2330 (6)	0.3909 (2)	0.0467 (9)
H11	0.4588	0.1017	0.4271	0.056*
C12	0.39688 (15)	0.2605 (6)	0.3370 (2)	0.0476 (9)
H12	0.3651	0.1477	0.3363	0.057*
C25	0.09958 (12)	0.8462 (5)	-0.19283 (18)	0.0311 (6)
H25A	0.1055	0.7968	-0.2504	0.037*
H25B	0.0775	0.9968	-0.1978	0.037*

C26	0.16362 (13)	0.8760 (5)	-0.13681 (18)	0.0290 (6)
C27	0.17905 (14)	1.0732 (5)	-0.0867 (2)	0.0333 (7)
H27	0.1497	1.1953	-0.0881	0.040*
C28	0.23634 (15)	1.0942 (6)	-0.0351 (2)	0.0422 (8)
H28	0.2446	1.2272	-0.0002	0.051*
C29	0.28176 (14)	0.9246 (6)	-0.0335 (2)	0.0387 (7)
C30	0.26777 (14)	0.7226 (6)	-0.0820 (2)	0.0447 (8)
H30	0.2978	0.6031	-0.0811	0.054*
C31	0.20875 (14)	0.6992 (6)	-0.1321 (2)	0.0408 (8)
H31	0.1992	0.5607	-0.1635	0.049*
C32	0.34424 (16)	0.9532 (6)	0.0221 (2)	0.0494 (9)
C50	0.05974 (12)	0.6632 (5)	-0.15437 (17)	0.0237 (6)
Co1	0.0000	0.5000	0.0000	0.02453 (15)
H5C	-0.0226 (18)	0.907 (7)	0.078 (3)	0.057 (13)*
H5D	-0.0072 (15)	0.719 (6)	0.134 (2)	0.049 (10)*
N1	0.09278 (10)	0.4435 (4)	0.07147 (14)	0.0278 (5)
N2	0.50139 (12)	0.3794 (5)	0.39444 (17)	0.0417 (6)
01	0.03952 (8)	0.7233 (3)	-0.08597 (11)	0.0252 (4)
O2	0.05249 (10)	0.4649 (4)	-0.18973 (14)	0.0392 (5)
O3	0.38617 (10)	0.7984 (4)	0.00934 (15)	0.0448 (6)
Н3	0.4191	0.8232	0.0426	0.067*
O4	0.35646 (11)	1.1161 (4)	0.07192 (15)	0.0506 (6)
05	-0.00449 (10)	0.7965 (4)	0.07875 (14)	0.0308 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0255 (14)	0.0263 (14)	0.0317 (15)	-0.0001 (11)	-0.0015 (11)	0.0051 (12)
C2	0.0228 (15)	0.0414 (18)	0.0314 (15)	0.0045 (12)	-0.0004 (12)	-0.0013 (13)
C3	0.0411 (17)	0.0279 (17)	0.052 (2)	-0.0034 (14)	-0.0078 (14)	0.0124 (15)
C4	0.0254 (14)	0.0280 (16)	0.0360 (16)	-0.0053 (11)	-0.0017 (12)	0.0017 (12)
C5	0.0329 (15)	0.0323 (17)	0.0372 (17)	-0.0017 (13)	-0.0112 (12)	0.0083 (13)
C6	0.0238 (16)	0.050 (2)	0.056 (2)	0.0032 (14)	-0.0049 (14)	0.0141 (17)
C7	0.0407 (18)	0.056 (2)	0.061 (2)	-0.0067 (18)	-0.0091 (15)	0.023 (2)
C8	0.0303 (16)	0.043 (2)	0.055 (2)	-0.0009 (14)	-0.0020 (13)	0.0019 (15)
C9	0.0383 (19)	0.050 (2)	0.053 (2)	-0.0036 (15)	-0.0021 (15)	0.0131 (17)
C10	0.0357 (17)	0.042 (2)	0.0446 (19)	-0.0083 (14)	-0.0035 (14)	-0.0042 (14)
C11	0.0469 (19)	0.0385 (19)	0.0453 (19)	-0.0024 (15)	-0.0222 (15)	0.0135 (15)
C12	0.0373 (18)	0.051 (2)	0.048 (2)	-0.0097 (16)	-0.0121 (15)	0.0094 (17)
C25	0.0254 (14)	0.0341 (17)	0.0340 (15)	-0.0005 (12)	0.0056 (12)	0.0059 (13)
C26	0.0241 (14)	0.0337 (16)	0.0301 (15)	-0.0018 (12)	0.0069 (11)	-0.0003 (12)
C27	0.0326 (16)	0.0210 (16)	0.0469 (18)	0.0048 (11)	0.0086 (13)	0.0006 (12)
C28	0.0408 (19)	0.0344 (18)	0.054 (2)	-0.0039 (14)	0.0135 (15)	-0.0099 (15)
C29	0.0296 (15)	0.044 (2)	0.0424 (17)	-0.0057 (13)	0.0056 (13)	-0.0033 (14)
C30	0.0256 (15)	0.052 (2)	0.054 (2)	0.0122 (15)	-0.0021 (13)	-0.0096 (17)
C31	0.0404 (17)	0.0326 (17)	0.0480 (19)	0.0022 (14)	0.0024 (14)	-0.0182 (14)
C32	0.0381 (18)	0.053 (2)	0.054 (2)	-0.0008 (16)	-0.0024 (15)	-0.0161 (18)
C50	0.0207 (12)	0.0236 (15)	0.0258 (13)	0.0028 (11)	0.0003 (10)	0.0029 (11)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Col	0.0260(3)	0 0223 (3)	0.0237(3)	0.0004(2)	0.00182(10)	0.0014(2)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N1	0.0207(3)	0.0223(3)	0.0237(3) 0.0307(12)	0.0004(2)	0.00132(17)	0.0014(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N2	0.0232(12) 0.0315(14)	0.0433 (16)	0.0461 (16)	0.0007(9)	-0.00000(12)	-0.0002(9)
$\begin{array}{cccccccc} 0.22 & 0.0491 (13) & 0.025 (12) & 0.0478 (13) & -0.0078 (10) & 0.0023 (10) & -0.0055 (9) \\ 0.3 & 0.0347 (12) & 0.0444 (14) & 0.0466 (13) & 0.0077 (11) & -0.0230 (10) & -0.0055 (9) \\ 0.0 & 0.0511 (15) & 0.0463 (14) & 0.0473 (14) & 0.0075 (11) & -0.0141 (11) & -0.0127 (12) \\ 0.0 & 0.0390 (11) & 0.0199 (11) & 0.0365 (12) & 0.0029 (9) & 0.0150 (9) & 0.0008 (9) \\ \hline \\ Geometric parameters (Å, °) \\ C1-C4 & 1.360 (4) & C25-H25A & 0.9700 \\ C1-H1 & 0.9300 & C26-C27 & 1.373 (4) \\ C2-C3 & 1.373 (4) & C26-C31 & 1.382 (4) \\ C2-C4 & 1.389 (4) & C27-C28 & 1.362 (4) \\ C2-C6 & 1.498 (4) & C27-H27 & 0.9300 \\ C3-C5 & 1.352 (4) & C28-C29 & 1.361 (4) \\ C3-H3A & 0.9300 & C28-H28 & 0.9300 \\ C4-H4 & 0.9300 & C29-C30 & 1.378 (5) \\ C5-N1 & 1.335 (4) & C29-C32 & 1.483 (4) \\ C5-H5A & 0.9300 & C30-C31 & 1.383 (4) \\ C6-C7 & 1.472 (5) & C30-H30 & 0.9300 \\ C7-C8 & 1.520 (4) & C32-O4 & 1.209 (4) \\ C7-H7 & 0.9300 & C32-O3 & 1.290 (4) \\ C7-H7 & 0.9300 & C32-O3 & 1.290 (4) \\ C7-H7 & 0.9300 & C32-O3 & 1.290 (4) \\ C8-C9 & 1.367 (5) & C50-O2 & 1.249 (3) \\ C8-C9 & 1.367 (5) & C50-O1 & 1.262 (3) \\ C9-C10 & 1.394 (4) & C01-O5 & 2.092 (2) \\ C10-N2 & 1.324 (4) & C01-O1 & 2.1149 (17) \\ C11-N2 & 1.303 (4) & C01-O5 & 2.092 (2) \\ C10-N2 & 1.378 (4) & C01-O1 & 2.1149 (17) \\ C11-H1 & 0.9300 & C31-H31 & 0.9300 \\ C25-C50 & 1.522 (4) & C32-C7-C26 & 1.249 (3) \\ C25-C26 & 1.514 (4) & C01-O1 & 2.1149 (17) \\ C11-H1 & 0.9300 & C01-O5 & 2.092 (2) \\ C10-N2 & 1.324 (4) & C01-O1 & 2.1149 (17) \\ C11-H1 & 0.9300 & C01-O5 & 0.908 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C26 & 1.514 (4) & 0.5-H5C & 0.73 (4) \\ C25-C2-C4 & 116 3 (3) & C29-C28-C37 & 1214 (3) \\ C3-C2-C4 & 116 3 (3) & C29-C28-C37 & 1214 (3) \\ C3-C2-C4 $	01	0.0313(14) 0.0242(9)	0.0455(10) 0.0268(10)	0.0761(10)	-0.0013(8)	0.0003 (8)	0.0018 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	02	0.0212(9) 0.0491(13)	0.0258(12)	0.0201(10) 0.0478(13)	-0.0078(10)	0.0033(0)	-0.0015(9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	03	0.0347(12)	0.0230(12) 0.0444(14)	0.0466 (13)	0.0077 (11)	-0.0200(10)	-0.0051(11)
O5 0.0390 (11) 0.0195 (12) 0.0029 (9) 0.0150 (9) 0.0008 (9) Geometric parameters $(\vec{A}, \vec{2})$ C1—N1 1.338 (3) C25—H25A 0.9700 C1—N1 1.336 (4) C25—H25B 0.9700 C1—H1 0.9300 C26—C27 1.373 (4) C2—C4 1.389 (4) C27—C28 1.352 (4) C2—C4 1.389 (4) C27—C28 1.361 (4) C3—H3A 0.9300 C28—H28 0.9300 C3—H3A 0.9300 C28—C30 1.378 (5) C5—N1 1.335 (4) C29—C30 1.378 (5) C5—H5A 0.9300 C30—H30 0.9300 C6—C7 1.472 (5) C30—H30 0.9300 C6—C7 1.472 (5) C30—H30 0.9300 C6=H6 0.9300 C32—O3 1.290 (4) C7—H7 0.9300 C32—O3 1.290 (4) C8=C9 1.367 (5) C50—O1 1.262 (3) C9—C10 1.394 (4) Co1—O5 2.092 (2) C9—C10<	04	0.0511 (15)	0.0463 (14)	0.0473 (14)	0.0075 (11)	-0.0141(11)	-0.0127(12)
Geometric parameters $(J, 9)$ Init (G) Init (G) <thini (g)<="" th=""> Init (G) <thin< td=""><td>05</td><td>0.0390 (11)</td><td>0.0199 (11)</td><td>0.0365 (12)</td><td>0.0029 (9)</td><td>0.0150 (9)</td><td>0.0008 (9)</td></thin<></thini>	05	0.0390 (11)	0.0199 (11)	0.0365 (12)	0.0029 (9)	0.0150 (9)	0.0008 (9)
Geometric parameters (Å. 9) C1—NI 1.338 (3) C25—H25A 0.9700 C1—C4 1.360 (4) C25—H25B 0.9700 C1—H1 0.9300 C26—C27 1.373 (4) C2—C3 1.373 (4) C26—C21 1.382 (4) C2—C4 1.389 (4) C27—H27 0.9300 C3—C5 1.352 (4) C28—C29 1.361 (4) C3—H3A 0.9300 C28—H28 0.9300 C4—H4 0.9300 C29—C30 1.378 (5) C5—N1 1.335 (4) C29—C31 1.383 (4) C6—C7 1.472 (5) C30—H30 0.9300 C6—H6 0.9300 C31—H31 0.9300 C7—H7 0.9300 C32—O4 1.209 (4) C7—H7 0.9300 C32—O3 1.290 (4) C8—C12 1.367 (5) C50—O1 1.262 (3) C9—C10 1.394 (4) Co1—O5 2.092 (2) C10—N2 1.367 (5) C50—O1 2.149 (3) C8—C9 1.367 (4) Co1—O5 2.092 (2) C9—H9 0.9300 Co1—O5 <			()				
C1-N1 1.338 (3) C25-H25A 0.9700 C1-C4 1.360 (4) C25-H25B 0.9700 C1-H1 0.9300 C26-C27 1.373 (4) C2-C3 1.373 (4) C26-C31 1.382 (4) C2-C4 1.389 (4) C27-C28 1.361 (4) C2-C5 1.352 (4) C28-C29 1.361 (4) C3-C5 1.352 (4) C29-C30 1.378 (5) C5-N1 1.335 (4) C29-C32 1.483 (4) C5-N1 1.335 (4) C29-C32 1.483 (4) C5-N1 1.335 (4) C29-C32 1.483 (4) C6-C7 1.472 (5) C30-H30 0.9300 C6-H6 0.9300 C31-H31 0.9300 C7-C8 1.520 (4) C32-O4 1.290 (4) C7-C8 1.520 (4) C32-O4 1.290 (4) C8-C9 1.367 (5) C50-O1 1.242 (3) C9-C10 1.394 (4) Co1-O5 2.092 (2) C1-M10 0.9300 Co1-O1 2.149 (17) C10-N2 1.378 (4) Co1-N1 2.149 (17)	Geometric param	neters (Å, °)					
C1-C41.360 (4)C25-H25B0.9700C1-H10.9300C26-C271.373 (4)C2-C31.373 (4)C26-C311.382 (4)C2-C41.389 (4)C27-C281.362 (4)C2-C61.498 (4)C27-H270.9300C3-C51.352 (4)C28-C291.361 (4)C3-H3A0.9300C28-H280.9300C4-H40.9300C29-C321.483 (4)C5N11.355 (4)C29-C321.483 (4)C5N11.355 (4)C29-C321.483 (4)C5FX0.9300C31-H310.9300C6-C71.472 (5)C30-H300.9300C6-C71.472 (5)C30-H310.9300C6-C71.472 (5)C30-O41.209 (4)C7-H70.9300C31-H310.9300C7-C81.520 (4)C32-O41.209 (4)C7-H70.9300C32-O31.290 (4)C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C10-N21.324 (4)Co1-O12.1149 (17)C10-N100.9300Co1-O12.1149 (17)C10-N100.9300Co1-O12.141 (2)C11-N21.303 (4)Co1-N1 i2.141 (2)C11-N21.303 (4)Co1-N1 i2.141 (2)C11-N10.9300C3-H5D0.98 (4)C25-C261.514 (4)0.5-H5D0.98 (4)C25-C261.514 (4)C5-H5D0.98 (4)C25-C261.522 (3)C28-C27	C1—N1		1.338 (3)	C2.	5—H25A	0.970	0
C1-H10.9300C26-C271.373 (4)C2-C31.373 (4)C26-C311.382 (4)C2-C41.389 (4)C27-C281.362 (4)C2-C61.498 (4)C27-H270.9300C3-C51.352 (4)C28-C291.361 (4)C3-H3A0.9300C28-H280.9300C4-H40.9300C29-C301.378 (5)C5-N11.335 (4)C29-C301.378 (5)C5-N11.335 (4)C29-C301.383 (4)C6-H60.9300C31-H310.9300C6-H60.9300C31-H310.9300C7-C81.520 (4)C32-O41.209 (4)C8-C121.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C9-H90.9300Co1-O5 ¹ 2.092 (2)C10-N100.9300Co1-O1 ¹ 2.1149 (17)C10-N100.9300Co1-O1 ¹ 2.141 (2)C11-N21.303 (4)Co1-N1 ¹ 2.141 (2)C11-N21.303 (4)Co1-N1 ¹ 2.141 (2)C11-C121.378 (4)Co1-N12.141 (2)C11-C120.9300C3-H5C0.73 (4)C25-C501.514 (4)C5-H5D0.98 (4)C25-C501.514 (3)C28-C27-C2612.5 (3)N1-C1-H1117.6C28-C27-H27119.2C3-C2-C4118.6 (3)C29-C28-C13119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6 <td>C1—C4</td> <td></td> <td>1.360 (4)</td> <td>C2.</td> <td>5—H25B</td> <td>0.970</td> <td>0</td>	C1—C4		1.360 (4)	C2.	5—H25B	0.970	0
$C2-C3$ 1.373 (4) $C26-C31$ 1.382 (4) $C2-C4$ 1.389 (4) $C27-C28$ 1.361 (4) $C2-C6$ 1.498 (4) $C27-H27$ 0.9300 $C3-C5$ 1.352 (4) $C28-C29$ 1.361 (4) $C3-H3A$ 0.9300 $C28-H28$ 0.9300 $C4-H4$ 0.9300 $C29-C30$ 1.378 (5) $C5-N1$ 1.335 (4) $C29-C32$ 1.483 (4) $C5-H5A$ 0.9300 $C30-C31$ 1.383 (4) $C6-C7$ 1.472 (5) $C30-H30$ 0.9300 $C6-H6$ 0.9300 $C31-H31$ 0.9300 $C7-C8$ 1.520 (4) $C32-O4$ 1.209 (4) $C7-H7$ 0.9300 $C32-O3$ 1.290 (4) $C8-C12$ 1.367 (5) $C50-O2$ 1.249 (3) $C8-C9$ 1.367 (5) $C50-O1$ 1.262 (3) $C9-C10$ 1.394 (4) $C01-O5^{1}$ 2.092 (2) $C10-N2$ 1.324 (4) $C01-O1^{1}$ 2.1149 (17) $C10-N2$ 1.303 (4) $C01-N1^{1}$ 2.1149 (17) $C11-N2$ 1.303 (4) $C01-N1^{1}$ 2.1149 (17) $C11-N1$ 0.9300 $Co1-N1^{1}$ 2.1149 (17) $C11-N2$ 1.378 (4) $C01-N1^{1}$ 2.1149 (17) $C11-N2$ 1.303 (4) $C01-N1^{1}$ 2.1149 (17) $C1-C1-H1$	C1—H1		0.9300	C2	6—C27	1.373	(4)
$C2-C4$ 1.389 (4) $C27-C28$ 1.362 (4) $C2-C6$ 1.498 (4) $C27-H27$ 0.9300 $C3-C5$ 1.352 (4) $C28-C29$ 1.361 (4) $C3-H13A$ 0.9300 $C29-C30$ 1.378 (5) $C5-N1$ 1.335 (4) $C29-C32$ 1.483 (4) $C5-H5A$ 0.9300 $C30-C31$ 1.383 (4) $C6-C7$ 1.472 (5) $C30-H30$ 0.9300 $C6-H6$ 0.9300 $C31-H31$ 0.9300 $C7-C8$ 1.520 (4) $C32-O4$ 1.209 (4) $C7-C8$ 1.520 (4) $C32-O3$ 1.290 (4) $C8-C9$ 1.367 (5) $C50-O2$ 1.249 (3) $C8-C9$ 1.367 (5) $C50-O1$ 1.262 (3) $C9-C10$ 1.394 (4) $C01-O5^{1}$ 2.092 (2) $C10-N2$ 1.324 (4) $C01-O1^{1}$ 2.1149 (17) $C11-N2$ 1.303 (4) $C01-O1^{1}$ 2.1149 (17) $C11-N2$ 1.378 (4) $C01-N1^{1}$ 2.1149 (17) $C11-N2$ 1.378 (4) $C01-N1^{1}$ 2.141 (2) $C11-N1$ 0.9300 $O3-H3$ 0.8200 $C2-C5$ 1.524 (3) $C28-C27-C26$ 215 (3) $NI-C1-C4$ 1248 (3) $C28-C27-H27$ 119.2 $C4-C1-H1$ 117.6 $C28-C27-H27$ 119.2 $C3-C2-C6$ 118.61 (3) $C29-C28-H28$ 119.3 $C4-C2-C6$ 125.03 $C27-C26-C32$ 125.03 $C3-C2-C6$ 118.63 $C29-C28-H28$ 119.3 $C4-C2-C6$ 125.03 </td <td>C2—C3</td> <td></td> <td>1.373 (4)</td> <td>C2</td> <td>6—C31</td> <td>1.382</td> <td>(4)</td>	C2—C3		1.373 (4)	C2	6—C31	1.382	(4)
$C2-C6$ 1.498 (4) $C27-H27$ 0.9300 $C3-C5$ 1.352 (4) $C28-C29$ 1.361 (4) $C3-H3A$ 0.9300 $C28-H28$ 0.9300 $C4-H4$ 0.9300 $C29-C30$ 1.378 (5) $C5-N1$ 1.335 (4) $C29-C32$ 1.483 (4) $C5-H5A$ 0.9300 $C30-C31$ 1.383 (4) $C6-C7$ 1.472 (5) $C30-H30$ 0.9300 $C7-C8$ 1.520 (4) $C32-O4$ 1.209 (4) $C7-H7$ 0.9300 $C32-O3$ 1.290 (4) $C8-C12$ 1.367 (5) $C50-O1$ 1.262 (3) $C9-C10$ 1.394 (4) $C01-O5$ 2.092 (2) $C9-H9$ 0.9300 $Ca1-O5^i$ 2.092 (2) $C9-H9$ 0.9300 $Ca1-O5^i$ 2.092 (2) $C10-N2$ 1.324 (4) $Co1-O1^i$ 2.1149 (17) $C10-N2$ 1.336 (4) $Co1-N1^i$ 2.1149 (17) $C1-H10$ 0.9300 $Ca1-O1^i$ 2.1149 (17) $C1-H11$ 0.9300 $C3-H5D$ 0.98 (4) $C25-C26$ 1.514 (4) $O5-H5D$ 0.98 (4) $C25-C26$ 1.514 (4) $O5-H5D$ 0.98 (4) $C25-C26$ 1.520 (3) $C28-C27-C26$ 12.15 (3) $N1-C1-H1$ 17.6 $C28-C27-H27$ 119.2 $C3-C2-C4$ 116.3 (3) $C29-C28-C27$ 12.14 (3) $C3-C2-C6$ 12.60 (3) $C27-C28-H28$ 119.3 $C5-C3-C2$ 12.08 (3) $C28-C29-C30$ 118.7 (3) $C2-C2-H3A$ 119.6 C	C2—C4		1.389 (4)	C2	7—С28	1.362	(4)
C3-C51.352 (4)C28-C291.361 (4)C3-H3A0.9300C28-H280.9300C4-H40.9300C29-C301.378 (5)C5-N11.335 (4)C29-C321.483 (4)C5-H5A0.9300C30-C311.383 (4)C6-C71.472 (5)C30-H300.9300C6-H60.9300C31-H310.9300C7-C81.520 (4)C32-O41.209 (4)C8-C121.367 (5)C50-O21.249 (3)C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C10-N21.324 (4)Co1-O5 ⁱ 2.092 (2)C10-N10.9300Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-N1 ⁱ 2.141 (2)C11-N21.303 (4)Co1-N1 ⁱ 2.141 (2)C11-H110.9300O3-H30.8200C12-C121.578 (4)Co1-N1 ⁱ 2.141 (2)C11-H110.9300O5-H5C0.73 (4)C25-C501.514 (4)O5-H5C0.73 (4)C25-C501.522 (4)IIN1-C1-C41248 (3)C28-C27-H27119.2N1-C1-H1117.6C26-C27-H27119.2C3-C2-C6118.6 (3)C29-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6125.0 (3)C28-C29-C30118.7 (3)C5-C3-C2120.8 (3)C28-C29-C32120.5 (3)C5-C3-C2120.8 (3)C28-C29-C32120.5 (3)C4-C2	C2—C6		1.498 (4)	C2	7—Н27	0.930	0
C3—H3A0.9300C28—H280.9300C4—H40.9300C29—C301.378 (5)C5—N11.335 (4)C29—C321.483 (4)C6—C71.472 (5)C30—H300.9300C6—H60.9300C31—H310.9300C7—C81.520 (4)C32—O41.209 (4)C8—C121.367 (5)C50—O21.249 (3)C8—C91.367 (5)C50—O11.262 (3)C9—C101.394 (4)Co1—O52.092 (2)C10—N21.324 (4)Co1—O52.092 (2)C10—N100.9300Co1—O12.1149 (17)C10—H100.9300Co1—O12.1149 (17)C11—N21.303 (4)Co1—N12.141 (2)C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C261.514 (4)O5—H5C0.73 (4)C25—C261.514 (3)C28—C27—C2612.15 (3)N1—C1—H1117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C2712.14 (3)C3—C2—C6125.0 (3)C27—C28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—C2120.8 (3)C28—C29—C32120.5 (3)C5—C3—C2120.8 (3)C28—C29—C32120.5 (3)C1—H1119.6C28—C29—C32120.5 (3)C2—C4119.6C28—C29—C32120.5 (3)C3—C2—C4119.6C28—C29—C32120.5 (3) <t< td=""><td>C3—C5</td><td></td><td>1.352 (4)</td><td>C2</td><td>8—C29</td><td>1.361</td><td>(4)</td></t<>	C3—C5		1.352 (4)	C2	8—C29	1.361	(4)
C4—H40.9300C29—C301.378 (5)C5—N11.335 (4)C29—C321.483 (4)C5—H5A0.9300C30—C311.383 (4)C6—C71.472 (5)C30—H300.9300C6—H60.9300C31—H310.9300C7—C81.520 (4)C32—O41.209 (4)C7—H70.9300C32—O31.290 (4)C8—C91.367 (5)C50—O21.249 (3)C8—C91.367 (5)C50—O11.262 (3)C9—C101.394 (4)Co1—O52.092 (2)C10—N21.324 (4)Co1—O1 ⁱ 2.1149 (17)C10—H100.9300Co1—O1 ⁱ 2.1149 (17)C11—N21.303 (4)Co1—N1 ⁱ 2.141 (2)C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C501.522 (4)VVN1—C1—C41248 (3)C28—C27—C26121.5 (3)N1—C1—H117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C4116.3 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—H3A119.6C30—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.5 (3)	С3—НЗА		0.9300	C2	8—H28	0.930	0
C5-N11.335 (4)C29-C321.483 (4)C5-H5A0.9300C30-C311.383 (4)C6-C71.472 (5)C30-H300.9300C6-H60.9300C31-H310.9300C7-C81.520 (4)C32-O41.290 (4)C7-H70.9300C32-O31.290 (4)C8-C121.367 (5)C50-O21.249 (3)C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C9-H90.9300Co1-O5 ⁱ 2.092 (2)C10-N11.324 (4)Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-O1 ⁱ 2.1149 (17)C11-N21.303 (4)Co1-N12.141 (2)C11-H110.9300O3-H30.8200C12-H120.9300O5-H5C0.73 (4)C25-C261.514 (4)O5-H5D0.98 (4)C25-C501.522 (4)117.6C28-C27-C26N1-C1-H1117.6C28-C27-H27119.2C4-C1-H1117.6C28-C27-H27119.2C3-C2-C4116.3 (3)C29-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C5-C3-H3A119.6C28-C29-C30118.7 (3)C5-C3-H3A119.6C28-C29-C32120.5 (3)C2-C3-H3A119.6C28-C29-C32120.5 (3)C2-C4-H27119.2 (3)C29-C38-C31119.5 (3)	C4—H4		0.9300	C2	9—С30	1.378	(5)
CS-H5A0.9300C30-C311.383 (4)C6-C71.472 (5)C30-H300.9300C6-H60.9300C31-H310.9300C7-C81.520 (4)C32-O41.209 (4)C7-H70.9300C32-O31.290 (4)C8-C121.367 (5)C50-O21.249 (3)C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C9-H90.9300Co1-O5 ⁱ 2.092 (2)C10-N21.324 (4)Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-O1 ⁱ 2.1149 (17)C11-H100.9300Co1-N1 ⁱ 2.141 (2)C11-H110.9300Co1-N1 ⁱ 2.141 (2)C11-H110.9300O3-H30.8200C12-H120.9300O3-H30.8200C12-H120.9300O5-H5C0.73 (4)C25-C261.514 (4)O5-H5D0.98 (4)C25-C501.522 (4)	C5—N1		1.335 (4)	C2	9—С32	1.483	(4)
$C6-C7$ $1.472 (5)$ $C30-H30$ 0.9300 $C6-H6$ 0.9300 $C31-H31$ 0.9300 $C7-C8$ $1.520 (4)$ $C32-O4$ $1.209 (4)$ $C7-H7$ 0.9300 $C32-O3$ $1.290 (4)$ $C8-C12$ $1.367 (5)$ $C50-O2$ $1.249 (3)$ $C8-C9$ $1.367 (5)$ $C50-O1$ $1.262 (3)$ $C9-C10$ $1.394 (4)$ $C01-O5$ $2.092 (2)$ $C9-H9$ 0.9300 $C01-O5^i$ $2.092 (2)$ $C10-N2$ $1.324 (4)$ $C01-O1^i$ $2.1149 (17)$ $C10-N1$ 0.9300 $C01-O1^i$ $2.1149 (17)$ $C10-H10$ 0.9300 $C01-O1^i$ $2.1149 (17)$ $C11-N2$ $1.303 (4)$ $C01-N1^i$ $2.141 (2)$ $C11-H11$ 0.9300 $03-H3$ 0.8200 $C12-H12$ 0.9300 $05-H5D$ $0.73 (4)$ $C25-C26$ $1.514 (4)$ $05-H5D$ $0.73 (4)$ $C25-C50$ $1.522 (4)$ V V $NI-C1-C4$ $124.8 (3)$ $C28-C27-C26$ $121.5 (3)$ $NI-C1-H11$ 117.6 $C26-C27-H27$ 119.2 $C3-C2-C4$ $116.3 (3)$ $C29-C28-H28$ 119.3 $C3-C2-C6$ $118.6 (3)$ $C29-C28-H28$ 119.3 $C4-C2-C6$ $125.0 (3)$ $C27-C28-H28$ 119.3 $C5-C3-H3A$ 119.6 $C28-C29-C30$ $118.7 (3)$ $C2-C3-H3A$ 119.6 $C29-C30-C31$ $119.5 (3)$	C5—H5A		0.9300	C3	0—C31	1.383	(4)
C6—H60.9300C31—H310.9300C7—C81.520 (4)C32—O41.209 (4)C7—H70.9300C32—O31.290 (4)C8—C121.367 (5)C50—O21.249 (3)C8—C91.367 (5)C50—O11.262 (3)C9—C101.394 (4)Co1—O52.092 (2)C9—H90.9300Co1—O5 ⁱ 2.092 (2)C10—N21.324 (4)Co1—O1 ⁱ 2.1149 (17)C10—H100.9300Co1—O1 ⁱ 2.1149 (17)C11—N21.303 (4)Co1—N12.141 (2)C11—C121.378 (4)Co1—N12.141 (2)C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C261.514 (4)O5—H5D0.98 (4)C25—C501.522 (4)VVN1—C1—C4124.8 (3)C28—C27—C26121.5 (3)N1—C1—H1117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C6125.0 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C29—C28—H28119.3C5—C3—H3A119.6C28—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	С6—С7		1.472 (5)	C3	0—Н30	0.930	0
C7-C8 1.520 (4)C32-O4 1.209 (4)C7-H70.9300C32-O3 1.290 (4)C8-C12 1.367 (5)C50-O2 1.249 (3)C8-C9 1.367 (5)C50-O1 1.262 (3)C9-C10 1.394 (4)Co1-O5 2.092 (2)C9-H90.9300Co1-O5 ⁱ 2.092 (2)C10-N2 1.324 (4)Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-O1 ⁱ 2.141 (2)C11-N2 1.303 (4)Co1-N1 ⁱ 2.141 (2)C11-C12 1.378 (4)Co1-N1 ⁱ 2.141 (2)C11-H110.9300O3-H30.8200C12-H120.9300O5-H5C0.73 (4)C25-C26 1.514 (4)O5-H5D0.98 (4)C25-C50 1.522 (4) 119.2 N1-C1-C4 124.8 (3)C28-C27-C26 121.5 (3)N1-C1-H1 117.6 C26-C27-H27 119.2 C3-C2-C4 116.3 (3)C29-C28-C27 121.4 (3)C3-C2-C5 118.6 (3)C29-C28-C27 121.4 (3)C3-C2-C6 125.0 (3)C27-C28-H28 119.3 C4-C2-C6 125.0 (3)C28-C29-C30 118.7 (3)C5-C3-H3A 119.6 C28-C29-C32 120.5 (3)C2-C3-H3A 119.6 C30-C29-C32 120.8 (3)C1-C4-C2 119.1 (3)C29-C30-C31 119.5 (3)	С6—Н6		0.9300	C3	1—Н31	0.930	0
C7-H70.9300C32-O31.290 (4)C8-C121.367 (5)C50-O21.249 (3)C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C9-H90.9300Co1-O1^i2.1149 (17)C10-N21.324 (4)Co1-O1^i2.1149 (17)C10-H100.9300Co1-O1^i2.1149 (17)C11-N21.303 (4)Co1-N1^i2.141 (2)C11-C121.378 (4)Co1-N12.141 (2)C11-H110.9300O3-H30.8200C12-H120.9300O5-H5C0.73 (4)C25-C261.514 (4)O5-H5D0.98 (4)C25-C501.522 (4)VVN1-C1-C4124.8 (3)C28-C27-C26121.5 (3)N1-C1-H1117.6C26-C27-H27119.2C3-C2-C4116.3 (3)C29-C28-C27121.4 (3)C3-C2-C5118.6 (3)C29-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6125.0 (3)C28-C29-C30118.7 (3)C5-C3-H3A119.6C28-C29-C32120.5 (3)C2-C23-H3A119.6C30-C29-C32120.8 (3)	С7—С8		1.520 (4)	C32	2—04	1.209	(4)
C8-C12 1.367 (5)C50-O2 1.249 (3)C8-C9 1.367 (5)C50-O1 1.262 (3)C9-C10 1.394 (4)Co1-O5 2.092 (2)C9-H9 0.9300 Co1-O5 ⁱ 2.092 (2)C10-N2 1.324 (4)Co1-O1 ⁱ 2.1149 (17)C10-H10 0.9300 Co1-O1 2.1149 (17)C11-N2 1.303 (4)Co1-N1 ⁱ 2.141 (2)C11-C12 1.378 (4)Co1-N1 2.141 (2)C11-H11 0.9300 O3-H3 0.8200 C12-H12 0.9300 O5-H5C 0.73 (4)C25-C26 1.514 (4)O5-H5D 0.98 (4)C25-C26 1.514 (4)O5-H5D 0.98 (4)C25-C50 1.522 (4) 119.2 N1-C1-H1 117.6 C28-C27-C26 121.5 (3)N1-C1-H1 117.6 C28-C27-H27 119.2 C4-C1-H1 117.6 C29-C28-C27 121.4 (3)C3-C2-C6 118.6 (3)C29-C28-C27 121.4 (3)C3-C2-C6 125.0 (3)C27-C28-H28 119.3 C4-C2-C6 125.0 (3)C27-C28-H28 119.3 C5-C3-H3A 119.6 C28-C29-C32 120.8 (3)C1-C4-C2 119.1 (3)C29-C30-C31 119.5 (3)	С7—Н7		0.9300	C3	2—ОЗ	1.290	(4)
C8-C91.367 (5)C50-O11.262 (3)C9-C101.394 (4)Co1-O52.092 (2)C9-H90.9300Co1-O5 ⁱ 2.092 (2)C10-N21.324 (4)Co1-O1 ⁱ 2.1149 (17)C10-H100.9300Co1-O12.1149 (17)C11-N21.303 (4)Co1-N1 ⁱ 2.141 (2)C11-C121.378 (4)Co1-N12.141 (2)C11-H110.9300O3-H30.8200C12-H120.9300O5-H5C0.73 (4)C25-C261.514 (4)O5-H5D0.98 (4)C25-C501.522 (4)VVN1-C1-C4124.8 (3)C28-C27-C26121.5 (3)N1-C1-H1117.6C26-C27-H27119.2C3-C2-C4116.3 (3)C29-C28-C27121.4 (3)C3-C2-C6118.6 (3)C29-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C5-C3-C2120.8 (3)C28-C29-C32120.5 (3)C5-C3-H3A119.6C30-C29-C32120.5 (3)C1-C4-C2119.1 (3)C29-C30-C31119.5 (3)	C8—C12		1.367 (5)	C5	0—О2	1.249	(3)
C9-C10 $1.394 (4)$ Co1-O5 $2.092 (2)$ C9-H9 0.9300 Co1-O5 ⁱ $2.092 (2)$ C10-N2 $1.324 (4)$ Co1-O1 ⁱ $2.1149 (17)$ C10-H10 0.9300 Co1-O1 $2.1149 (17)$ C11-N2 $1.303 (4)$ Co1-N1 ⁱ $2.141 (2)$ C11-C12 $1.378 (4)$ Co1-N1 $2.141 (2)$ C11-H11 0.9300 O3-H3 0.8200 C12-H12 0.9300 O5-H5C $0.73 (4)$ C25-C26 $1.514 (4)$ O5-H5D $0.98 (4)$ C25-C50 $1.522 (4)$ 119.2 N1-C1-C4 $124.8 (3)$ $C28-C27-C26$ $121.5 (3)$ N1-C1-H1 117.6 $C29-C28-C27$ 119.2 C4-C1-H1 $116.3 (3)$ $C29-C28-C27$ $121.4 (3)$ C3-C2-C6 $118.6 (3)$ $C29-C28-H28$ 119.3 C4-C2-C6 $125.0 (3)$ $C27-C28-H28$ 119.3 C5-C3-C2 $120.8 (3)$ $C28-C29-C30$ $118.7 (3)$ C5-C3-H3A 119.6 $C28-C29-C32$ $120.5 (3)$ C1-C4-C2 $119.1 (3)$ $C29-C30-C31$ $119.5 (3)$	С8—С9		1.367 (5)	C5	0—O1	1.262	(3)
C9—H90.9300 $C_{01}-O5^i$ 2.092 (2)C10—N21.324 (4) $C_{01}-O1^i$ 2.1149 (17)C10—H100.9300 $C_{01}-O1$ 2.1149 (17)C11—N21.303 (4) $C_{01}-N1^i$ 2.141 (2)C11-C121.378 (4) $C_{01}-N1^i$ 2.141 (2)C11-H110.930003-H30.8200C12-H120.930005-H5C0.73 (4)C25-C261.514 (4)05-H5D0.98 (4)C25-C501.522 (4) V V N1-C1-C4124.8 (3)C28-C27-C26121.5 (3)N1-C1-H1117.6C28-C27-H27119.2C4-C1-H1117.6C29-C28-C27121.4 (3)C3-C2-C6118.6 (3)C29-C28-H28119.3C4-C2-C6125.0 (3)C27-C28-H28119.3C4-C2-C6125.0 (3)C28-C29-C30118.7 (3)C5-C3-H3A119.6C28-C29-C32120.5 (3)C2-C3-H3A119.6C30-C29-C32120.8 (3)C1-C4-C2119.1 (3)C29-C30-C31119.5 (3)	C9—C10		1.394 (4)	Co	1—05	2.092	(2)
C10—N2 $1.324 (4)$ Co1—O1 ⁱ $2.1149 (17)$ C10—H100.9300Co1—O1 $2.1149 (17)$ C11—N2 $1.303 (4)$ Co1—N1 ⁱ $2.141 (2)$ C11—C12 $1.378 (4)$ Co1—N1 $2.141 (2)$ C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C26 $1.514 (4)$ O5—H5D0.98 (4)C25—C50 $1.522 (4)$ $1.522 (4)$ $1.92 (24) (24) (24) (24) (24) (25) (26) (26) (26) (26) (26) (26) (26) (26$	С9—Н9		0.9300	Со	1—05 ⁱ	2.092	(2)
C10—H100.9300Co1—O12.1149 (17)C11—N21.303 (4)Co1—N1 i 2.141 (2)C11—C121.378 (4)Co1—N12.141 (2)C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C261.514 (4)O5—H5D0.98 (4)C25—C501.522 (4)	C10—N2		1.324 (4)	Co	1—01 ⁱ	2.114	9 (17)
C11—N21.303 (4) C_{01} —N12.141 (2)C11—C121.378 (4)Co1—N12.141 (2)C11—H110.9300O3—H30.8200C12—H120.9300O5—H5C0.73 (4)C25—C261.514 (4)O5—H5D0.98 (4)C25—C501.522 (4)VN1—C1—C4124.8 (3)C28—C27—C26121.5 (3)N1—C1—H1117.6C28—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C6118.6 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—H3A119.6C30—C29—C32120.5 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	C10—H10		0.9300	Co	1—01	2.114	9 (17)
$\begin{array}{cccccccc} C11C12 & 1.378 (4) & Co1N1 & 2.141 (2) \\ C11H11 & 0.9300 & O3H3 & 0.8200 \\ C12H12 & 0.9300 & O5H5C & 0.73 (4) \\ C25C26 & 1.514 (4) & O5H5D & 0.98 (4) \\ C25C50 & 1.522 (4) & & & \\ N1C1C4 & 124.8 (3) & C28C27C26 & 121.5 (3) \\ N1C1H1 & 117.6 & C28C27H27 & 119.2 \\ C4C1H1 & 117.6 & C26C27H27 & 119.2 \\ C3C2C4 & 116.3 (3) & C29C28C27 & 121.4 (3) \\ C3C2C6 & 118.6 (3) & C29C28H28 & 119.3 \\ C4C2C6 & 125.0 (3) & C27C28H28 & 119.3 \\ C4C2C6 & 125.0 (3) & C28C29C30 & 118.7 (3) \\ C5C3H3A & 119.6 & C28C29C32 & 120.8 (3) \\ C2C3H3A & 119.6 & C30C29C32 & 120.8 (3) \\ C1C4C2 & 119.1 (3) & C29C30C31 & 119.5 (3) \\ \end{array}$	C11—N2		1.303 (4)	Co	1—N1 ⁱ	2.141	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—C12		1.378 (4)	Co	1—N1	2.141	(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C11—H11		0.9300	03	—Н3	0.820	0
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12—H12		0.9300	05	—Н5С	0.73	(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C25—C26		1.514 (4)	05	—H5D	0.98	(4)
N1—C1—C4124.8 (3)C28—C27—C26121.5 (3)N1—C1—H1117.6C28—C27—H27119.2C4—C1—H1117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C6118.6 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—H3A119.6C28—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	C25—C50		1.522 (4)				
N1—C1—H1117.6C28—C27—H27119.2C4—C1—H1117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C6118.6 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—H3A119.6C28—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	N1—C1—C4		124.8 (3)	C2	8—C27—C26	121.5	(3)
C4—C1—H1117.6C26—C27—H27119.2C3—C2—C4116.3 (3)C29—C28—C27121.4 (3)C3—C2—C6118.6 (3)C29—C28—H28119.3C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—H3A119.6C28—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	N1—C1—H1		117.6	C2	8—С27—Н27	119.2	
C3-C2-C4116.3 (3) $C29-C28-C27$ 121.4 (3) $C3-C2-C6$ 118.6 (3) $C29-C28-H28$ 119.3 $C4-C2-C6$ 125.0 (3) $C27-C28-H28$ 119.3 $C5-C3-C2$ 120.8 (3) $C28-C29-C30$ 118.7 (3) $C5-C3-H3A$ 119.6 $C28-C29-C32$ 120.5 (3) $C2-C3-H3A$ 119.6 $C30-C29-C32$ 120.8 (3) $C1-C4-C2$ 119.1 (3) $C29-C30-C31$ 119.5 (3)	C4—C1—H1		117.6	C2	6—С27—Н27	119.2	
C3-C2-C6 118.6 (3) C29-C28-H28 119.3 C4-C2-C6 125.0 (3) C27-C28-H28 119.3 C5-C3-C2 120.8 (3) C28-C29-C30 118.7 (3) C5-C3-H3A 119.6 C28-C29-C32 120.5 (3) C2-C3-H3A 119.6 C30-C29-C32 120.8 (3) C1-C4-C2 119.1 (3) C29-C30-C31 119.5 (3)	C3—C2—C4		116.3 (3)	C2	9—C28—C27	121.4	(3)
C4—C2—C6125.0 (3)C27—C28—H28119.3C5—C3—C2120.8 (3)C28—C29—C30118.7 (3)C5—C3—H3A119.6C28—C29—C32120.5 (3)C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	C3—C2—C6		118.6 (3)	C2	9—С28—Н28	119.3	
C5-C3-C2120.8 (3)C28-C29-C30118.7 (3)C5-C3-H3A119.6C28-C29-C32120.5 (3)C2-C3-H3A119.6C30-C29-C32120.8 (3)C1-C4-C2119.1 (3)C29-C30-C31119.5 (3)	C4—C2—C6		125.0 (3)	C2	7—С28—Н28	119.3	
C5-C3-H3A119.6C28-C29-C32120.5 (3)C2-C3-H3A119.6C30-C29-C32120.8 (3)C1-C4-C2119.1 (3)C29-C30-C31119.5 (3)	C5—C3—C2		120.8 (3)	C2	8—C29—C30	118.7	(3)
C2—C3—H3A119.6C30—C29—C32120.8 (3)C1—C4—C2119.1 (3)C29—C30—C31119.5 (3)	С5—С3—НЗА		119.6	C2	8—C29—C32	120.5	(3)
C1—C4—C2 119.1 (3) C29—C30—C31 119.5 (3)	С2—С3—НЗА		119.6	C3	0—C29—C32	120.8	(3)
	C1—C4—C2		119.1 (3)	C2	9—C30—C31	119.5	(3)

C1—C4—H4	120.5	C29—C30—H30	120.3
C2—C4—H4	120.5	C31—C30—H30	120.3
N1—C5—C3	124.0 (3)	C26—C31—C30	121.8 (3)
N1—C5—H5A	118.0	C26—C31—H31	119.1
С3—С5—Н5А	118.0	C30—C31—H31	119.1
C7—C6—C2	117.1 (3)	O4—C32—O3	122.1 (3)
С7—С6—Н6	121.4	O4—C32—C29	123.0 (3)
С2—С6—Н6	121.4	O3—C32—C29	114.7 (3)
C6—C7—C8	115.2 (3)	O2—C50—O1	125.6 (2)
С6—С7—Н7	122.4	O2—C50—C25	118.2 (2)
С8—С7—Н7	122.4	O1—C50—C25	116.1 (2)
С12—С8—С9	117.1 (3)	O5—Co1—O5 ⁱ	180.00 (10)
C12—C8—C7	124.0 (3)	O5—Co1—O1 ⁱ	92.48 (8)
C9—C8—C7	118.9 (3)	O5 ⁱ —Co1—O1 ⁱ	87.52 (8)
C8—C9—C10	119.4 (3)	O5—Co1—O1	87.52 (8)
С8—С9—Н9	120.3	O5 ⁱ —Co1—O1	92.48 (8)
С10—С9—Н9	120.3	O1 ⁱ —Co1—O1	180.00 (7)
N2—C10—C9	122.9 (3)	O5—Co1—N1 ⁱ	93.70 (9)
N2—C10—H10	118.5	O5 ⁱ —Co1—N1 ⁱ	86.30 (9)
С9—С10—Н10	118.5	O1 ⁱ —Co1—N1 ⁱ	89.61 (8)
N2-C11-C12	124.1 (3)	O1—Co1—N1 ⁱ	90.39 (8)
N2-C11-H11	117.9	O5—Co1—N1	86.30 (9)
C12—C11—H11	117.9	O5 ⁱ —Co1—N1	93.70 (9)
C8—C12—C11	119.6 (3)	O1 ⁱ —Co1—N1	90.39 (8)
C8—C12—H12	120.2	O1—Co1—N1	89.61 (8)
C11—C12—H12	120.2	N1 ⁱ —Co1—N1	180.00 (13)
C26—C25—C50	110.9 (2)	C5—N1—C1	115.0 (2)
C26—C25—H25A	109.5	C5—N1—Co1	122.57 (19)
С50—С25—Н25А	109.5	C1—N1—Co1	122.36 (19)
С26—С25—Н25В	109.5	C11—N2—C10	116.8 (3)
С50—С25—Н25В	109.5	C50—O1—Co1	127.08 (17)
H25A—C25—H25B	108.1	С32—О3—Н3	109.5
C27—C26—C31	117.0 (3)	Co1—O5—H5C	138 (3)
C27—C26—C25	122.4 (3)	Co1—O5—H5D	100 (2)
C31—C26—C25	120.6 (3)	H5C—O5—H5D	107 (3)
Symmetry codes: (i) $-x$, $-y+1$, $-z$.			
Hydrogen-bond geometry (Å. °)			

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	D—H··· A
O5—H5C···O1 ⁱⁱ	0.73 (4)	2.13 (4)	2.822 (3)	158 (4)
O5—H5D···O2 ⁱ	0.98 (4)	1.74 (4)	2.610 (3)	145 (3)
O3—H3···N2 ⁱⁱⁱ	0.82	1.85	2.667 (3)	173.
0 = 1 = 1 = 1 = 1 = 1 = 1 = 1 = 1 = 1 =		1/2		

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



Fig. 1



