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Bis[μ-(2-carboxylatoethyl)phosphonato]-bis[aqua(2,2′-bipyridine)cobalt(II)]

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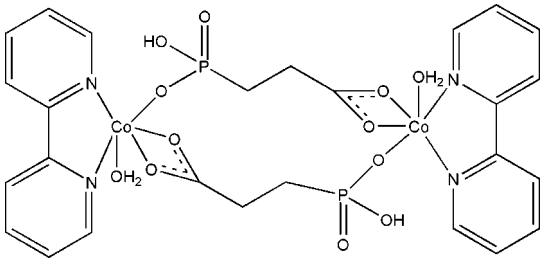
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.029; wR factor = 0.070; data-to-parameter ratio = 18.9.

The title compound, $[Co_2(HO_3PCH_2CH_2COO)_2(C_{10}H_8N_2)_2(H_2O)_2]$, was obtained by a hydrothermal method. Two six-coordinate cobalt(II) ions are linked by two 2-carboxyethylphosphonate ligands, forming a centrosymmetric dimer. The dimers are further interlinked by O—H···O hydrogen bonds and π–π stacking [centroid–centroid distance = 4.2975 (5) Å] to form a three-dimensional supramolecular structure. The compound is isostructural with the analogous zinc(II) complex reported recently [Ying, Li, Chen, Liu & Liu (2007). *Acta Cryst.* E**63**, m555–m557].

Related literature

For related literature, see: Clearfield (1998); Cheetham *et al.* (1999); Stock *et al.* (2000); Serpaggi & Férey (1999); Ying & Mao (2004); Ying *et al.* (2006, 2007).



Experimental

Crystal data

$[Co_2(C_3H_5O_5P)_2(C_{10}H_8N_2)_2(H_2O)_2]$
M_r = 770.34
Orthorhombic, *Pbca*
a = 8.6384 (18) Å
b = 17.701 (4) Å
c = 20.619 (4) Å
V = 3152.8 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.22 mm^{-1}
T = 293 (2) K
0.34 × 0.33 × 0.06 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.682, T_{max} = 0.930
22346 measured reflections
3924 independent reflections
2241 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.070
S = 0.78
3924 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6B···O4^{i}	0.82	1.93	2.7198 (19)	163
O1—H1B···O3^{ii}	0.82	1.72	2.533 (2)	169

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: RZ2168).

References

Bruker (2004). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cheetham, A. K., Férey, G. & Loiseau, T. (1999). *Angew. Chem. Int. Ed.* **38**, 3268–3292.
Clearfield, A. (1998). *Progress in Inorganic Chemistry*, Vol. 47, edited by K. D. Karlin, pp. 371–510. New York: John Wiley & Sons Inc.
Serpaggi, F. & Férey, G. (1999). *Inorg. Chem.* **38**, 4741–4744.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.
Stock, N., Frey, S. A., Stucky, G. D. & Cheetham, A. K. (2000). *J. Chem. Soc. Dalton Trans.* pp. 4292–4296.
Ying, S.-M., Li, X.-F., Chen, W.-T., Liu, D.-S. & Liu, J.-H. (2007). *Acta Cryst.* E**63**, m555–m557.
Ying, S.-M. & Mao, J.-G. (2004). *Eur. J. Inorg. Chem.* pp. 1270–1276.
Ying, S.-M., Zeng, X.-R., Fang, X.-N., Li, X.-F. & Liu, D.-S. (2006). *Inorg. Chim. Acta*, **359**, 1589–1593.

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supplementary materials

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Bis[μ-(2-carboxylatoethyl)phosphonato]bis[aqua(2,2'-bipyridine)cobalt(II)]

S.-M. Ying, Y. Chen, J.-Y. Lin, G.-P. Zhou and J.-H. Wu

Comment

Recently, the chemistry of metal phosphonates has been a research field of rapid expansion, mainly due to their potential application in the area of catalysis, ion exchange, proton conductivity, intercalation chemistry, photochemistry and material chemistry (Clearfield 1998). Many metal phosphonates have been reported (Cheetham *et al.*, 1999; Stock *et al.*, 2000; Serpaggi & Férey, 1999; Ying & Mao, 2004; Ying *et al.*, 2006). The metal phosphonates can exhibit various kinds of structure. We report here the crystal structure of a new cobalt(II) carboxyalkylphosphonate complex synthesized by the hydrothermal method.

The asymmetric unit of the title compound contains one cobalt(II) ion, one doubly deprotonated 2-carboxyethylphosphonic acid ligand, one 2,2'-bipyridine and one coordinated water molecule. The cobalt(II) ion is six-coordinated by one phosphonate oxygen atom, one water molecule, two carboxylate oxygen atoms and two N atoms of a 2,2'-bipyridine molecule. The Co—O distances range from 2.0076 (13) to 2.2112 (15) Å and the Co—N distances are 2.1038 (16) and 2.1471 (17) Å. Two cobalt(II) ions are linked by two 2-carboxyethylphosphonic acid ligands forming a dimer (Fig. 1). The dimers are further interlinked by O—H···O hydrogen bonds (Table 1) and π-π stacking interactions to form a three-dimensional supermolecular structure (Fig. 2). The compound is isostructural with the analogous zinc(II) complex reported recently (Ying *et al.*, 2007).

Experimental

A mixture of cobalt(II) acetate (0.5 mmol, 0.123 g), 2-carboxyethylphosphonic acid (0.5 mmol, 0.078 g), and 2,2'-bipyridine (0.5 mmol, 0.078 g) in 10 ml of distilled water was sealed in an autoclave equipped with a Teflon liner (20 ml) and then heated at 160°C for 4 days. Crystals of the title compound were obtained.

Refinement

All hydrogen atoms were positioned geometrically and with C—H = 0.93–0.98 Å, O—H = 0.82 Å, and refined in the riding-model approximation, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(O).

Figures

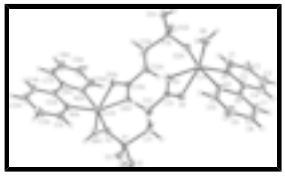

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (A) 2 − *x*, 1 − *y*, 1 − *z*.]

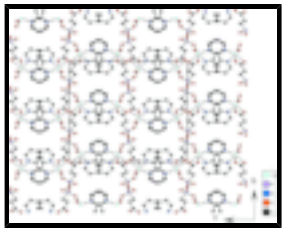

Fig. 2. Packing diagram of the title compound viewed along the *a* axis. Hydrogen atoms are omitted for clarity.

Bis[μ-(2-carboxylatoethyl)phosphonato]bis[aqua(2,2'-bipyridine)cobalt(II)]

Crystal data

$[Co_2(C_3H_5O_5P_1)_2(C_{10}H_8N_2)_2(H_2O)_2]$	F_{000} = 1576
M_r = 770.34	D_x = 1.623 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 7543 reflections
a = 8.6384 (18) Å	θ = 2.3–28.2º
b = 17.701 (4) Å	μ = 1.22 mm^{-1}
c = 20.619 (4) Å	*T* = 293 (2) K
V = 3152.8 (11) Å^3	Plate, pink
Z = 4	0.34 × 0.33 × 0.06 mm

Data collection

Bruker APEX area-detector diffractometer	3924 independent reflections
Radiation source: fine-focus sealed tube	2241 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 293(2) K	θ_{max} = 28.4º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	*h* = −11→10
T_{min} = 0.682, T_{max} = 0.930	*k* = −23→23
22346 measured reflections	*l* = −26→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained
$wR(F^2)$ = 0.070	$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.78	$(\Delta/\sigma)_{max}$ = 0.025
3924 reflections	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = −0.53 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.67017 (3)	0.427251 (15)	0.405818 (12)	0.02945 (9)
P1	1.15669 (6)	0.69676 (3)	0.49404 (3)	0.03041 (14)
N1	0.7003 (2)	0.38302 (10)	0.31196 (8)	0.0380 (5)
N2	0.5524 (2)	0.50685 (9)	0.34466 (8)	0.0379 (4)
O5	0.87439 (17)	0.50256 (8)	0.40645 (6)	0.0410 (4)
O4	0.69834 (16)	0.51179 (8)	0.48183 (7)	0.0383 (4)
O3	1.05769 (16)	0.76527 (7)	0.50687 (7)	0.0429 (4)
O2	1.21917 (16)	0.66098 (7)	0.55427 (6)	0.0360 (4)
O1	1.28912 (17)	0.71919 (8)	0.44566 (7)	0.0428 (4)
H1B	1.3711	0.7228	0.4654	0.064*
O6	0.45576 (15)	0.39234 (7)	0.43781 (6)	0.0386 (4)
H6B	0.4259	0.4205	0.4668	0.046*
H6A	0.4103	0.3516	0.4199	0.046*
C13	0.8227 (2)	0.53500 (11)	0.45580 (10)	0.0308 (5)
C12	0.9046 (2)	0.60169 (12)	0.48543 (10)	0.0382 (5)
H12A	0.9347	0.5885	0.5293	0.046*
H12B	0.8321	0.6434	0.4882	0.046*
C11	1.0474 (2)	0.62845 (11)	0.44921 (10)	0.0390 (5)
H11A	1.0159	0.6505	0.4082	0.047*
H11B	1.1129	0.5853	0.4398	0.047*
C5	0.6405 (3)	0.42324 (12)	0.26241 (9)	0.0389 (5)
C6	0.5562 (3)	0.49213 (12)	0.28068 (10)	0.0380 (5)
C4	0.6598 (3)	0.39995 (15)	0.19871 (11)	0.0565 (7)
H4A	0.6182	0.4282	0.1649	0.068*
C10	0.4766 (3)	0.56851 (13)	0.36431 (11)	0.0539 (7)
H10A	0.4737	0.5787	0.4085	0.065*
C7	0.4842 (3)	0.53934 (15)	0.23605 (11)	0.0552 (7)
H7A	0.4881	0.5285	0.1919	0.066*
C1	0.7808 (3)	0.31957 (13)	0.29949 (11)	0.0504 (7)
H1A	0.8227	0.2921	0.3337	0.060*
C3	0.7403 (4)	0.33528 (16)	0.18596 (13)	0.0680 (9)

H3A	0.7531	0.3190	0.1434	0.082*
C9	0.4028 (3)	0.61769 (14)	0.32318 (12)	0.0667 (8)
H9A	0.3516	0.6601	0.3390	0.080*
C8	0.4071 (3)	0.60219 (16)	0.25800 (12)	0.0672 (8)
H8A	0.3579	0.6342	0.2287	0.081*
C2	0.8023 (3)	0.29448 (15)	0.23620 (14)	0.0652 (8)
H2A	0.8580	0.2506	0.2280	0.078*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03229 (17)	0.02827 (15)	0.02781 (14)	−0.00034 (13)	0.00030 (13)	−0.00079 (12)
P1	0.0257 (3)	0.0270 (3)	0.0385 (3)	−0.0013 (2)	−0.0008 (3)	0.0023 (2)
N1	0.0425 (13)	0.0365 (11)	0.0351 (10)	−0.0059 (9)	0.0035 (9)	−0.0090 (9)
N2	0.0425 (12)	0.0410 (11)	0.0302 (10)	0.0029 (9)	−0.0015 (8)	0.0016 (8)
O5	0.0475 (11)	0.0392 (9)	0.0362 (8)	−0.0118 (7)	0.0076 (7)	−0.0070 (7)
O4	0.0339 (10)	0.0326 (8)	0.0485 (9)	−0.0061 (7)	0.0075 (7)	−0.0067 (7)
O3	0.0304 (9)	0.0276 (8)	0.0708 (10)	0.0049 (6)	0.0001 (8)	0.0038 (7)
O2	0.0374 (9)	0.0327 (8)	0.0379 (8)	0.0052 (7)	−0.0020 (7)	0.0039 (7)
O1	0.0335 (10)	0.0529 (10)	0.0420 (9)	−0.0100 (7)	0.0022 (7)	0.0050 (8)
O6	0.0352 (9)	0.0345 (8)	0.0461 (9)	−0.0045 (7)	0.0035 (7)	−0.0085 (7)
C13	0.0313 (13)	0.0255 (11)	0.0355 (12)	0.0000 (10)	−0.0047 (10)	0.0036 (9)
C12	0.0304 (13)	0.0368 (12)	0.0476 (13)	−0.0056 (10)	0.0026 (11)	−0.0064 (10)
C11	0.0398 (15)	0.0394 (13)	0.0380 (12)	−0.0098 (10)	−0.0028 (10)	0.0009 (10)
C5	0.0422 (15)	0.0463 (13)	0.0281 (11)	−0.0168 (11)	−0.0001 (9)	−0.0049 (11)
C6	0.0378 (14)	0.0436 (13)	0.0326 (12)	−0.0115 (11)	−0.0038 (10)	0.0028 (10)
C4	0.081 (2)	0.0582 (16)	0.0306 (13)	−0.0185 (15)	0.0051 (13)	−0.0086 (12)
C10	0.0689 (19)	0.0539 (15)	0.0389 (13)	0.0184 (14)	−0.0041 (12)	0.0003 (12)
C7	0.0644 (19)	0.0675 (17)	0.0336 (13)	−0.0051 (15)	−0.0102 (12)	0.0079 (13)
C1	0.0569 (18)	0.0458 (15)	0.0485 (15)	−0.0023 (13)	0.0051 (12)	−0.0138 (12)
C3	0.094 (2)	0.070 (2)	0.0392 (15)	−0.0225 (18)	0.0194 (16)	−0.0194 (15)
C9	0.081 (2)	0.0611 (18)	0.0577 (18)	0.0288 (16)	−0.0069 (16)	0.0063 (14)
C8	0.078 (2)	0.0700 (19)	0.0533 (17)	0.0161 (17)	−0.0152 (16)	0.0185 (15)
C2	0.072 (2)	0.0529 (17)	0.071 (2)	−0.0049 (14)	0.0217 (16)	−0.0284 (15)

Geometric parameters (Å, °)

Co1—O2^{i}	2.0076 (13)	C12—H12A	0.9700
Co1—O6	2.0610 (14)	C12—H12B	0.9700
Co1—N1	2.1038 (16)	C11—H11A	0.9700
Co1—N2	2.1471 (17)	C11—H11B	0.9700
Co1—O4	2.1806 (14)	C5—C4	1.387 (3)
Co1—O5	2.2112 (15)	C5—C6	1.469 (3)
P1—O2	1.4948 (14)	C6—C7	1.390 (3)
P1—O3	1.5074 (14)	C4—C3	1.365 (3)
P1—O1	1.5690 (15)	C4—H4A	0.9300
P1—C11	1.791 (2)	C10—C9	1.373 (3)
N1—C5	1.348 (3)	C10—H10A	0.9300

N1—C1	1.346 (3)	C7—C8	1.373 (3)
N2—C10	1.336 (3)	C7—H7A	0.9300
N2—C6	1.345 (3)	C1—C2	1.391 (3)
O5—C13	1.251 (2)	C1—H1A	0.9300
O4—C13	1.269 (2)	C3—C2	1.372 (4)
O2—Co1^{i}	2.0076 (13)	C3—H3A	0.9300
O1—H1B	0.8200	C9—C8	1.372 (3)
O6—H6B	0.8200	C9—H9A	0.9300
O6—H6A	0.9000	C8—H8A	0.9300
C13—C12	1.506 (3)	C2—H2A	0.9300
C12—C11	1.517 (3)		
O2^{i}—Co1—O6	93.64 (6)	C13—C12—H12B	108.5
O2^{i}—Co1—N1	91.64 (6)	C11—C12—H12B	108.5
O6—Co1—N1	107.10 (6)	H12A—C12—H12B	107.5
O2^{i}—Co1—N2	167.65 (6)	C12—C11—P1	112.65 (14)
O6—Co1—N2	87.65 (6)	C12—C11—H11A	109.1
N1—Co1—N2	76.26 (7)	P1—C11—H11A	109.1
O2^{i}—Co1—O4	100.73 (6)	C12—C11—H11B	109.1
O6—Co1—O4	94.36 (5)	P1—C11—H11B	109.1
N1—Co1—O4	154.52 (6)	H11A—C11—H11B	107.8
N2—Co1—O4	91.42 (6)	N1—C5—C4	121.0 (2)
O2^{i}—Co1—O5	94.97 (6)	N1—C5—C6	115.71 (17)
O6—Co1—O5	153.62 (5)	C4—C5—C6	123.3 (2)
N1—Co1—O5	97.53 (6)	N2—C6—C7	121.5 (2)
N2—Co1—O5	89.19 (6)	N2—C6—C5	115.10 (19)
O4—Co1—O5	59.54 (5)	C7—C6—C5	123.4 (2)
O2—P1—O3	113.57 (8)	C3—C4—C5	119.5 (2)
O2—P1—O1	111.85 (8)	C3—C4—H4A	120.2
O3—P1—O1	108.76 (8)	C5—C4—H4A	120.2
O2—P1—C11	109.46 (9)	N2—C10—C9	124.0 (2)
O3—P1—C11	109.55 (10)	N2—C10—H10A	118.0
O1—P1—C11	103.13 (9)	C9—C10—H10A	118.0
C5—N1—C1	119.60 (19)	C8—C7—C6	119.1 (2)
C5—N1—Co1	116.95 (14)	C8—C7—H7A	120.5
C1—N1—Co1	123.39 (16)	C6—C7—H7A	120.5
C10—N2—C6	117.89 (19)	N1—C1—C2	121.0 (2)
C10—N2—Co1	126.17 (14)	N1—C1—H1A	119.5
C6—N2—Co1	115.94 (14)	C2—C1—H1A	119.5
C13—O5—Co1	89.81 (12)	C4—C3—C2	119.7 (2)
C13—O4—Co1	90.73 (12)	C4—C3—H3A	120.2
P1—O2—Co1^{i}	147.36 (9)	C2—C3—H3A	120.2
P1—O1—H1B	109.5	C8—C9—C10	117.8 (2)
Co1—O6—H6B	109.5	C8—C9—H9A	121.1
Co1—O6—H6A	120.0	C10—C9—H9A	121.1
H6B—O6—H6A	130.5	C7—C8—C9	119.9 (2)
O5—C13—O4	119.84 (19)	C7—C8—H8A	120.1
O5—C13—C12	121.47 (19)	C9—C8—H8A	120.1

O4—C13—C12	118.69 (18)	C3—C2—C1	119.2 (3)
C13—C12—C11	115.28 (18)	C3—C2—H2A	120.4
C13—C12—H12A	108.5	C1—C2—H2A	120.4
C11—C12—H12A	108.5		

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6B···O4^{ii}	0.82	1.93	2.7198 (19)	163
O1—H1B···O3^{iii}	0.82	1.72	2.533 (2)	169

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

Fig. 1

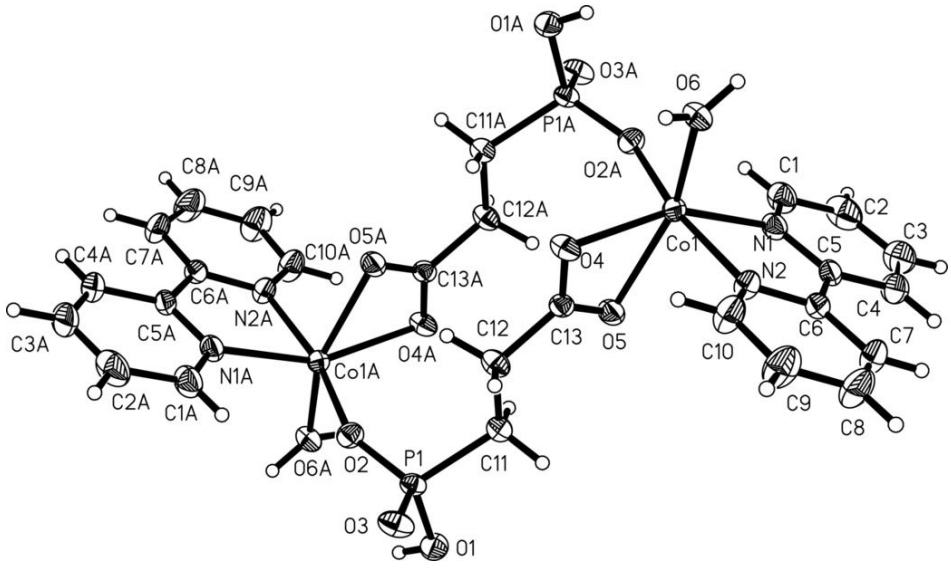
O1A
O3A
O6
C11A
P1A
O2A
C1
C8A
C9A
C12A
C2
C3
O5A
C10A
C7A
C4A
C13A
O4
Co1
N1
C5
N2
C6A
C4
C6
C3A
N2A
C5A
C12
C13
O5
C7
C10
O4A
Co1A
N1A
C2A
C1A
C9
C8
O6A
O2
P1
C11
O3
O1

Fig. 2