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catena-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-κO]cobalt(II)]-μ-4,4′-bipyridine-$\kappa^2N:N'$]

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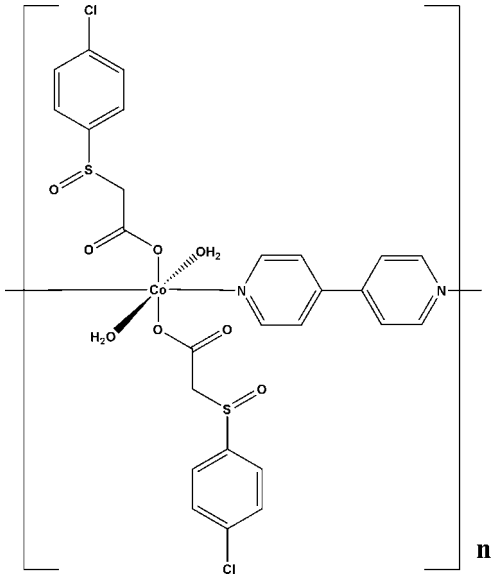
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.081; data-to-parameter ratio = 17.2.

In the title coordination polymer, $[Co(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]_n$, the Co^{II} atom exists in an octahedral coordination environment formed by two carboxylate O atoms from two (4-chlorophenylsulfinyl)acetate ligands, two N atoms from bipyridine ligands and two water molecules. The Co^{II} atom lies on a twofold rotation axis. Bridging by the bipyridine ligand leads to a linear chain structure, and intermolecular O—H···O hydrogen bonds link the chains into a three-dimensional network.

Related literature

For related literature, see: Ghosh *et al.* (2005); Nobles & Thompson (1965).



Experimental

Crystal data

$[Co(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$
M_r = 686.42
Orthorhombic, *Fdd*2
a = 20.129 (4) Å
b = 25.466 (5) Å
c = 11.413 (2) Å
V = 5850 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.96 mm^{-1}
T = 293 (2) K
0.27 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.782, T_{max} = 0.839
14081 measured reflections
3237 independent reflections
2728 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.081
S = 1.04
3237 reflections
188 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), with 1480 Friedel pairs
Flack parameter: −0.021 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H12···O1^{i}	0.85	1.87	2.692 (3)	164
O4—H12···S2^{i}	0.85	2.98	3.806 (2)	165
O4—H11···O2^{ii}	0.85	1.84	2.651 (3)	159

Symmetry codes: (i) $x+\frac{1}{4}, -y+\frac{7}{4}, z-\frac{1}{4}$; (ii) $-x, -y+2, z$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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: *SHELXL97*.

The authors thank Heilongjiang University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2260).

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supplementary materials

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catena-Poly[[diaquabis[(4-chlorophenylsulfinyl)acetato-*κO*]cobalt(II)]-*μ*-4,4'-bipyridine-*κ*^{2}*N*:*N*']

Y.-J. Hou, Y.-H. Yu, Z.-Z. Sun, B.-Y. Li and G.-F. Hou

Comment

4,4'-Bipyridine and organic aromatic carboxylic acid ligands are often used to bridge metal atoms and these compounds can demonstrate various network topologies (Ghosh *et al.*, 2005). The title compound, (I), is a cobalt(II) 4-chlorophenylsulfinylacetate that is bridged by 4,4'-bipyridine into a linear chain. The Co^{II} atom shows an all-*trans* octahedral coordination. The chains are connected into a three-dimensional network *via* intermolecular O—H···O hydrogen bonds (Table 1, Fig. 2).

Experimental

(4-Chlorophenylsulfanyl)acetic acid was prepared by nucleophilic reaction of chloroacetic acid and 4-chlorothiophenol under basic conditions. It was then oxidized using 30% aqueous hydrogen peroxide in acetic anhydride solution to produce 4-chlorophenylsulfinyl acetic acid (Nobles & Thompson, 1965). Cobalt nitrate hexahydrate (0.582 g, 2 mmol), 4,4'-bipyridine (0.312 g, 2 mmol) and 4-chlorophenylsulfinyl acetic acid (0.437 g, 2 mmol) were dissolved in water and the pH was adjusted to 6 with 0.01 *M* sodium hydroxide. Pink crystals separated from the filtered solution after several days.

Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C) or C—H = 0.97 Å (methylene C), and with U_{iso}(H) = 1.2U_{eq}(C). Water H atoms were initially located in a difference Fourier map but they were treated as riding on their parent atoms with O—H = 0.85 Å and with U_{iso}(H) = 1.5U_{eq}(O).

Figures

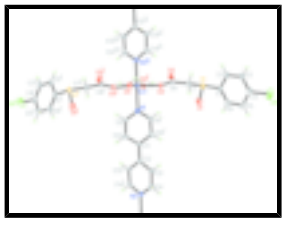


Fig. 1. Part of the polymeric structure of the title complex, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii. [Symmetry codes: (I) −*x*, −*y* + 2, *z*; (II) *x*, *y*,*z* − 1; (III) −*x*, −*y* + 2, *z* − 1; (IV) *x*, *y*, *z* + 1].

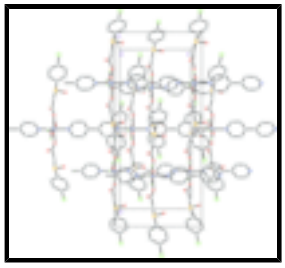


Fig. 2. A partial packing plot of (I). Dashed lines indicate the hydrogen-bonding interactions. H atoms not involved in hydrogen bonds have been omitted.

catena-Poly[[[diaquabis[(4-chlorophenylsulfinyl)acetato-\ κ*O*]cobalt(II)]-μ-4,4'-bipyridine-κ^2*N*:*N*']]

Crystal data

$[Co(C_8H_6ClO_3S)_2(C_{10}H_8N_2)(H_2O)_2]$	F_{000} = 2808
M_r = 686.42	D_x = 1.559 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 10618 reflections
a = 20.129 (4) Å	θ = 6.3–54.9º
b = 25.466 (5) Å	μ = 0.96 mm^{-1}
c = 11.413 (2) Å	*T* = 293 (2) K
V = 5850 (2) Å^3	Block, brown
Z = 8	0.27 × 0.25 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	3237 independent reflections
Radiation source: fine-focus sealed tube	2728 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.064
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −26→26
T_{min} = 0.782, T_{max} = 0.839	*k* = −32→32
14081 measured reflections	*l* = −14→14

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 12.1874P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.081	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
3237 reflections	$\Delta\rho_{min}$ = −0.33 e Å^{-3}

188 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: none

Absolute structure: Flack (1983), with how many Friedel pairs?

Flack parameter: −0.021 (18)

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}
C1	0.02753 (18)	0.72535 (12)	0.2402 (3)	0.0328 (8)
C2	0.06450 (19)	0.70613 (13)	0.1485 (3)	0.0388 (8)
H1	0.0606	0.7214	0.0747	0.047*
C3	0.1071 (2)	0.66474 (13)	0.1647 (4)	0.0479 (10)
H2	0.1332	0.6523	0.1035	0.058*
C4	0.1099 (2)	0.64239 (14)	0.2734 (4)	0.0496 (10)
C5	0.0737 (2)	0.66005 (17)	0.3665 (4)	0.0541 (11)
H3	0.0768	0.6440	0.4395	0.065*
C6	0.0322 (2)	0.70276 (15)	0.3487 (3)	0.0469 (10)
H4	0.0074	0.7161	0.4107	0.056*
C7	0.02917 (17)	0.82876 (11)	0.1972 (3)	0.0367 (8)
H5	0.0573	0.8307	0.2661	0.044*
H6	0.0572	0.8214	0.1300	0.044*
C8	−0.00637 (19)	0.88119 (11)	0.1794 (3)	0.0329 (8)
C9	0.0204 (2)	1.04139 (13)	0.4480 (3)	0.0408 (9)
H7	0.0358	1.0706	0.4072	0.049*
C10	0.0198 (2)	1.04325 (15)	0.5685 (4)	0.0463 (10)
H8	0.0329	1.0737	0.6071	0.056*
C11	0.0000	1.0000	0.6319 (4)	0.0331 (13)
C12	0.0000	1.0000	0.7620 (5)	0.0362 (14)
C13	0.0337 (2)	0.96238 (15)	0.8246 (3)	0.0403 (9)
H9	0.0567	0.9359	0.7858	0.048*
C14	0.03323 (19)	0.96414 (13)	0.9455 (3)	0.0391 (9)
H10	0.0574	0.9389	0.9863	0.047*
Cl1	0.16178 (8)	0.58814 (6)	0.29368 (16)	0.0944 (5)
N1	0.0000	1.0000	0.3873 (3)	0.0291 (10)
N2	0.0000	1.0000	1.0066 (3)	0.0330 (11)

O1	−0.06217 (15)	0.78760 (10)	0.3313 (3)	0.0570 (8)
O2	−0.06390 (14)	0.88010 (10)	0.1425 (3)	0.0515 (7)
O3	0.02768 (11)	0.92078 (8)	0.2029 (2)	0.0332 (5)
O4	0.10051 (11)	1.02305 (8)	0.19801 (19)	0.0357 (5)
H12	0.1238	1.0058	0.1493	0.054*
H11	0.0992	1.0555	0.1808	0.054*
S2	−0.03025 (5)	0.77720 (3)	0.21482 (9)	0.0379 (2)
Co1	0.0000	1.0000	0.19793 (4)	0.02525 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0347 (19)	0.0281 (15)	0.035 (2)	−0.0017 (14)	0.0055 (15)	−0.0014 (15)
C2	0.045 (2)	0.0334 (17)	0.0378 (18)	0.0034 (16)	0.0094 (17)	0.0062 (16)
C3	0.051 (3)	0.0378 (19)	0.055 (2)	0.0070 (17)	0.0152 (19)	−0.0029 (19)
C4	0.043 (2)	0.0368 (19)	0.068 (3)	0.0051 (18)	−0.006 (2)	0.0122 (19)
C5	0.060 (3)	0.060 (3)	0.042 (2)	0.004 (2)	0.001 (2)	0.025 (2)
C6	0.057 (3)	0.048 (2)	0.036 (2)	0.0026 (19)	0.0103 (18)	0.0008 (18)
C7	0.0383 (18)	0.0291 (15)	0.0428 (19)	0.0013 (13)	0.0046 (18)	0.0000 (16)
C8	0.043 (2)	0.0268 (14)	0.028 (2)	−0.0018 (15)	0.0017 (16)	0.0010 (14)
C9	0.065 (3)	0.0351 (18)	0.0219 (18)	−0.0124 (17)	−0.0059 (17)	0.0031 (15)
C10	0.073 (3)	0.036 (2)	0.030 (2)	−0.0120 (19)	−0.0086 (19)	−0.0009 (16)
C11	0.042 (4)	0.045 (3)	0.012 (3)	−0.003 (2)	0.000	0.000
C12	0.051 (4)	0.033 (3)	0.025 (3)	−0.006 (2)	0.000	0.000
C13	0.055 (3)	0.045 (2)	0.0208 (18)	0.0106 (18)	0.0064 (17)	−0.0022 (16)
C14	0.049 (2)	0.0390 (19)	0.029 (2)	0.0093 (16)	0.0014 (18)	0.0023 (16)
Cl1	0.0814 (11)	0.0679 (8)	0.1339 (14)	0.0381 (7)	−0.0058 (9)	0.0272 (9)
N1	0.036 (3)	0.036 (2)	0.015 (2)	0.0017 (17)	0.000	0.000
N2	0.043 (3)	0.037 (2)	0.019 (2)	0.0003 (19)	0.000	0.000
O1	0.0551 (19)	0.0439 (15)	0.072 (2)	0.0013 (13)	0.0340 (16)	−0.0001 (15)
O2	0.0508 (18)	0.0356 (13)	0.0683 (18)	0.0025 (12)	−0.0212 (15)	−0.0091 (12)
O3	0.0443 (13)	0.0252 (10)	0.0300 (11)	−0.0013 (9)	−0.0008 (12)	0.0005 (10)
O4	0.0400 (13)	0.0332 (10)	0.0338 (11)	0.0043 (9)	0.0046 (11)	0.0019 (12)
S2	0.0343 (5)	0.0284 (4)	0.0511 (5)	−0.0009 (3)	0.0013 (4)	−0.0024 (4)
Co1	0.0340 (3)	0.0249 (3)	0.0169 (2)	0.0013 (3)	0.000	0.000

Geometric parameters (Å, °)

C1—C6	1.369 (5)	C10—H8	0.9300
C1—C2	1.374 (5)	C11—C10^{i}	1.377 (5)
C1—S2	1.783 (3)	C11—C12	1.484 (5)
C2—C3	1.371 (5)	C12—C13	1.375 (4)
C2—H1	0.9300	C12—C13^{i}	1.375 (4)
C3—C4	1.366 (6)	C13—C14	1.381 (5)
C3—H2	0.9300	C13—H9	0.9300
C4—C5	1.364 (6)	C14—N2	1.330 (4)
C4—Cl1	1.747 (4)	C14—H10	0.9300
C5—C6	1.387 (6)	N1—C9^{i}	1.326 (4)

C5—H3	0.9300	N1—Co1	2.161 (4)
C6—H4	0.9300	N2—C14^{i}	1.330 (4)
C7—C8	1.528 (4)	N2—Co1^{ii}	2.183 (4)
C7—S2	1.787 (3)	O1—S2	1.500 (3)
C7—H5	0.9700	O3—Co1	2.094 (2)
C7—H6	0.9700	O4—Co1	2.107 (2)
C8—O2	1.232 (4)	O4—H12	0.8498
C8—O3	1.248 (4)	O4—H11	0.8502
C9—N1	1.326 (4)	Co1—O3^{i}	2.094 (2)
C9—C10	1.376 (6)	Co1—O4^{i}	2.107 (2)
C9—H7	0.9300	Co1—N2^{iii}	2.183 (4)
C10—C11	1.377 (5)		
C6—C1—C2	120.1 (3)	C13—C12—C11	121.3 (2)
C6—C1—S2	120.2 (3)	C13^{i}—C12—C11	121.3 (2)
C2—C1—S2	119.6 (3)	C12—C13—C14	119.6 (4)
C3—C2—C1	120.6 (3)	C12—C13—H9	120.2
C3—C2—H1	119.7	C14—C13—H9	120.2
C1—C2—H1	119.7	N2—C14—C13	123.4 (3)
C4—C3—C2	118.0 (4)	N2—C14—H10	118.3
C4—C3—H2	121.0	C13—C14—H10	118.3
C2—C3—H2	121.0	C9—N1—C9^{i}	117.0 (4)
C5—C4—C3	123.2 (4)	C9—N1—Co1	121.5 (2)
C5—C4—Cl1	118.5 (3)	C9^{i}—N1—Co1	121.5 (2)
C3—C4—Cl1	118.3 (3)	C14^{i}—N2—C14	116.7 (4)
C4—C5—C6	117.8 (4)	C14^{i}—N2—Co1^{ii}	121.6 (2)
C4—C5—H3	121.1	C14—N2—Co1^{ii}	121.6 (2)
C6—C5—H3	121.1	C8—O3—Co1	128.8 (2)
C1—C6—C5	120.2 (4)	Co1—O4—H12	112.6
C1—C6—H4	119.9	Co1—O4—H11	103.9
C5—C6—H4	119.9	H12—O4—H11	111.7
C8—C7—S2	110.1 (2)	O1—S2—C1	105.45 (17)
C8—C7—H5	109.6	O1—S2—C7	104.87 (16)
S2—C7—H5	109.6	C1—S2—C7	97.23 (16)
C8—C7—H6	109.6	O3^{i}—Co1—O3	176.87 (13)
S2—C7—H6	109.6	O3^{i}—Co1—O4^{i}	90.73 (8)
H5—C7—H6	108.2	O3—Co1—O4^{i}	89.26 (8)
O2—C8—O3	127.4 (3)	O3^{i}—Co1—O4	89.26 (8)
O2—C8—C7	117.8 (3)	O3—Co1—O4	90.73 (8)
O3—C8—C7	114.8 (3)	O4^{i}—Co1—O4	179.95 (15)
N1—C9—C10	123.2 (3)	O3^{i}—Co1—N1	88.43 (6)
N1—C9—H7	118.4	O3—Co1—N1	88.43 (6)
C10—C9—H7	118.4	O4^{i}—Co1—N1	89.98 (6)
C9—C10—C11	120.0 (4)	O4—Co1—N1	89.98 (6)
C9—C10—H8	120.0	O3^{i}—Co1—N2^{iii}	91.57 (6)
C11—C10—H8	120.0	O3—Co1—N2^{iii}	91.57 (6)

C10—C11—C10^{i}	116.6 (5)	O4^{i}—Co1—N2^{iii}	90.02 (6)
C10—C11—C12	121.7 (2)	O4—Co1—N2^{iii}	90.02 (6)
C10^{i}—C11—C12	121.7 (2)	N1—Co1—N2^{iii}	180.000 (2)
C13—C12—C13^{i}	117.3 (5)		

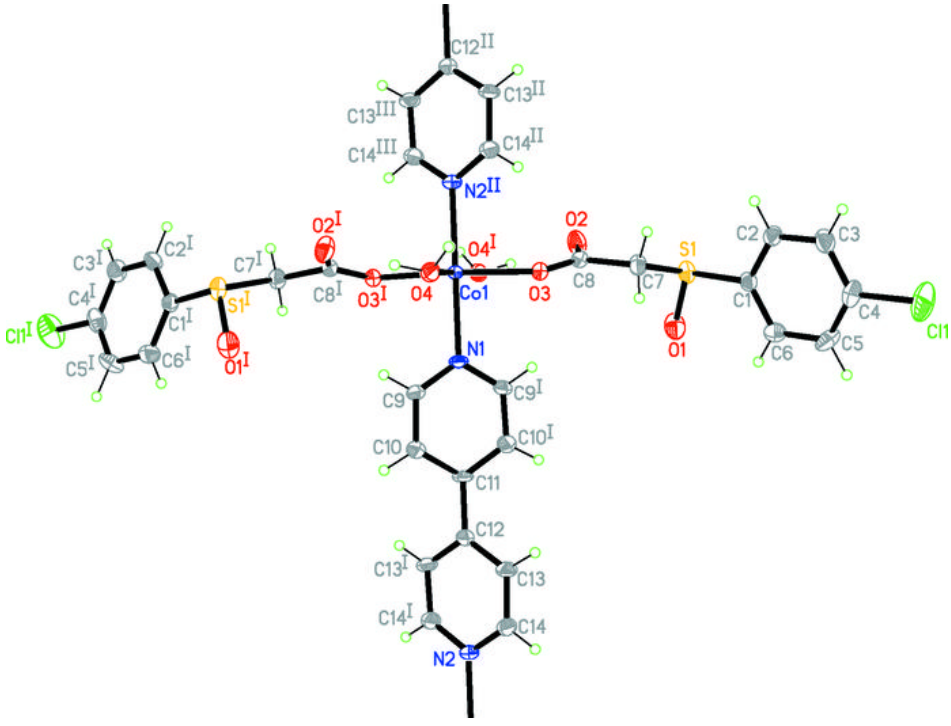
Symmetry codes: (i) −*x*, −*y*+2, *z*; (ii) *x*, *y*, *z*+1; (iii) *x*, *y*, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H12···O1^{iv}	0.85	1.87	2.692 (3)	164
O4—H12···S2^{iv}	0.85	2.98	3.806 (2)	165
O4—H11···O2^{i}	0.85	1.84	2.651 (3)	159

Symmetry codes: (iv) *x*+1/4, −*y*+7/4, *z*−1/4; (i) −*x*, −*y*+2, *z*.

Fig. 1


C12II
C13II
C13III
C14II
C14III
N2II
O2I
O4I
O2
S1
C2
C3
C7I
C2I
C3I
C4I
S1I
C8I
O3I
O4
Co1
O3
C8
C7
C1
C4
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O1
C6
C5
C5I
C6I
N1
C9I
C9
C10I
C10
C11
C12
C13I
C13
C14I
C14
N2

Fig. 2