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catena-Poly[[dichloridocobalt(II)]-μ-1,3-di-4-pyridylpropane-κ^2N:N']

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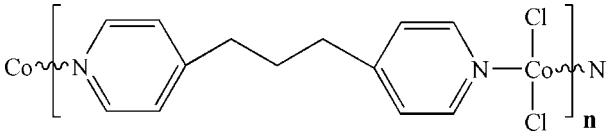
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.099; data-to-parameter ratio = 19.1.

In the title compound, $[CoCl_2(C_{13}H_{14}N_2)]_n$, 1,3-bis(4-pyridyl)-propane (bpp) ligands bridge four-coordinate Co atoms, generating an extended one-dimensional zigzag chain. Both the Co and two Cl atoms in the tetrahedral coordination polyhedron lie on a mirror plane, while the bbp ligand is bisected through the central C atom in the chain by a second mirror plane. There are some π–π stacking interations in the crystal structure, with interplanar distances of 3.449 Å, which are responsible for the supramolecular assembly.

Related literature

For related literature, see: Batten *et al.* (1999); Chen *et al.* (2004); Grosshans *et al.* (2004); Lee *et al.* (2004); Maji *et al.* (2005); Niu *et al.* (2003); Paz & Klinowski (2004); Carlucci *et al.* (1997); Pan *et al.* (2001).



Experimental

Crystal data

$[CoCl_2(C_{13}H_{14}N_2)]$
M_r = 328.09
Monoclinic, $P2_1/m$
a = 5.1899 (10) Å
b = 12.989 (3) Å
c = 10.490 (2) Å
β = 93.58 (3)°
V = 705.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 295 (2) K
0.36 × 0.25 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.628, T_{max} = 0.813
6891 measured reflections
1678 independent reflections
1307 reflections with $I > 2\sigma(I)$
R_{int} = 0.057

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.098
S = 1.03
1678 reflections
88 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—N1	2.034 (2)	Co1—Cl2	2.2539 (14)
Co1—Cl1	2.2400 (14)		

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2192).

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supplementary materials

Acta Cryst. (2008). E**64**, m1025 [**doi:10.1107/S1600536808020862**]

catena-Poly[[dichloridocobalt(II)]-μ-1,3-di-4-pyridylpropane-κ^2N:N']

W. Xu and J.-L. Lin

Comment

Transition metal complexes with the flexible ligand 1,3-bis(4-pyridyl)propane (bpp) have been investigated extensively (Pan, *et al.*, 2001; Batten, *et al.*, 1999; Carlucci, *et al.*, 1997; Lee, *et al.*, 2004), and some of these compounds have potential application in nonlinear optical (NLO), magnetic, gas adsorption and microporous materials (Maji, *et al.*, 2005; Niu, *et al.*, 2003; Paz, *et al.*, 2004). Our interest in transition metal-bpp complexes prompted us to report a new bpp-containing complex, $[Co(bpp)Cl_2]_n$, (I), obtained by self-assembly from $CoCl_2$ and bpp in DMF solution. It is isostructural with the previously reported complex $[Zn(bpp)Cl_2]_n$ (Chen, *et al.*, 2004).

In the title compound, the Co atom is coordinated by two N atoms of two bpp ligands and two Cl anions, forming a distorted tetrahedron (Figure 1 and Table 1.) Both the cation and two chlorine atoms in the coordination polyhedra lie on a mirror plane, while the bbp ligand is bisected through the central carbon in the chain by a second mirror. The angles around Co(II) ions span the range 104.2° to 125. 7°. The Co—N bond distance is 2.034 (2) Å, and the Co—Cl distances are 2.240 (1) and 2.254 (1) Å, similar to those found in other related structures (Grosshans, *et al.*, 2004). The bpp ligand is in a TT conformation, with a dihedral angle between two pyridine rings of 64.9°, and a C5—C6—C7—C6^{i} (i = -*x*, 1.5 - *y*, *z*) torsion angle of 176.0°. Each bpp ligand bridges two cobalt(II) ions together *via* nitrogen atoms to form one-dimensional zigzag chains; there are π-π interations between pyridine rings, which are arranged in a face-to-face fashion with interplanar distances of 3.449 Å.

Experimental

Addition of 1,3-bis(4-pyridyl)propane (bpp) (0.198 g, 1.0 mmol) to a stirred DMF solution (30 ml) of $CoCl_2.6H_2O$ (0.207 g 1.0 mmol) yielded a purple precipitate, which was refluxed for 30 min at 423 K followed by filtration after cooling. The resulting blue filtrate was maintained at room temperature; slow evaporation afforded a small amount of purple platelet cystals 15 days later (yield: 42% based on the initial $CoCl_2.6H_2O$ input).

Refinement

All H atoms werer located theoretically and refined as riding atoms, with C—H distances in the range 0.93–0.97 Å and $U_{iso}(H) = 1.2\ U_{eq}(C)$.

Figures

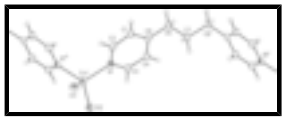

Fig. 1. *ORTEP* view of the title compound. The dispalcement ellipsoids are drawn at 40% probability level.

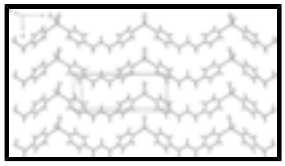

Fig. 2. The crystal packing of the title complex, view pallel to (001).

catena-Poly[[dichloridocobalt(II)]-μ-1,3-di-4-pyridylpropane- $\kappa^2N:N'$]

Crystal data

$[CoCl_2(C_{13}H_{14}N_2)]$	F_{000} = 334
M_r = 328.09	D_x = 1.544 Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yb	Cell parameters from 4916 reflections
a = 5.1899 (10) Å	θ = 3.1–27.5º
b = 12.989 (3) Å	μ = 1.58 mm^{-1}
c = 10.490 (2) Å	T = 295 (2) K
β = 93.58 (3)º	Palte, purple
V = 705.8 (3) Å^3	0.36 × 0.25 × 0.13 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	1678 independent reflections
Radiation source: fine-focus sealed tube	1307 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.057
Detector resolution: 0 pixels mm^{-1}	θ_{max} = 27.5º
T = 295(2) K	θ_{min} = 3.1º
ω scans	h = −6→6
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −16→16
T_{min} = 0.628, T_{max} = 0.813	l = −13→13
6891 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.098	$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.5699P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
1678 reflections	$\Delta\rho_{max}$ = 0.56 e Å^{-3}
88 parameters	$\Delta\rho_{min}$ = −0.32 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	0.45224 (11)	0.2500	0.72216 (5)	0.0469 (2)
Cl1	0.5449 (2)	0.2500	0.51643 (11)	0.0644 (3)
Cl2	0.7429 (2)	0.2500	0.89105 (11)	0.0563 (3)
N1	0.2438 (5)	0.38105 (17)	0.7418 (2)	0.0456 (5)
C1	−0.1030 (6)	0.4919 (2)	0.6704 (3)	0.0541 (8)
H1A	−0.2369	0.5056	0.6097	0.065*
C2	0.0502 (6)	0.4066 (2)	0.6576 (3)	0.0543 (8)
H2A	0.0175	0.3645	0.5867	0.065*
C3	0.2864 (6)	0.4443 (2)	0.8422 (3)	0.0515 (7)
H3A	0.4195	0.4283	0.9025	0.062*
C4	0.1436 (6)	0.5310 (2)	0.8601 (3)	0.0528 (7)
H4A	0.1821	0.5727	0.9309	0.063*
C5	−0.0580 (6)	0.5572 (2)	0.7735 (3)	0.0463 (7)
C6	−0.2140 (6)	0.6529 (2)	0.7913 (3)	0.0523 (7)
H6A	−0.2666	0.6554	0.8784	0.063*
H6B	−0.3688	0.6506	0.7346	0.063*
C7	−0.0613 (8)	0.7500	0.7639 (4)	0.0476 (9)
H7A	−0.0195	0.7500	0.6750	0.057*
H7B	0.0993	0.7500	0.8163	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0569 (4)	0.0384 (3)	0.0452 (3)	0.000	0.0009 (3)	0.000
Cl1	0.0673 (7)	0.0813 (8)	0.0442 (6)	0.000	0.0004 (5)	0.000
Cl2	0.0634 (7)	0.0500 (6)	0.0539 (6)	0.000	−0.0076 (5)	0.000
N1	0.0506 (13)	0.0385 (11)	0.0474 (14)	−0.0043 (11)	0.0002 (11)	0.0027 (10)
C1	0.0570 (17)	0.0463 (16)	0.0573 (19)	−0.0023 (15)	−0.0108 (15)	0.0018 (13)
C2	0.0651 (19)	0.0453 (16)	0.0514 (18)	−0.0055 (15)	−0.0057 (15)	−0.0044 (13)
C3	0.0586 (18)	0.0419 (15)	0.0528 (18)	0.0007 (14)	−0.0070 (14)	−0.0038 (12)
C4	0.0604 (18)	0.0430 (15)	0.0541 (18)	−0.0034 (15)	−0.0029 (14)	−0.0070 (13)

C5	0.0475 (15)	0.0373 (14)	0.0545 (17)	−0.0088 (12)	0.0053 (13)	0.0040 (12)
C6	0.0515 (16)	0.0409 (15)	0.065 (2)	−0.0007 (14)	0.0092 (15)	0.0043 (13)
C7	0.050 (2)	0.0363 (19)	0.057 (3)	0.000	0.0068 (19)	0.000

Geometric parameters (Å, °)

Co1—N1^{i}	2.034 (2)	C3—H3A	0.9300
Co1—N1	2.034 (2)	C4—C5	1.385 (4)
Co1—Cl1	2.2400 (14)	C4—H4A	0.9300
Co1—Cl2	2.2539 (14)	C5—C6	1.501 (4)
N1—C2	1.338 (4)	C6—C7	1.526 (4)
N1—C3	1.343 (4)	C6—H6A	0.9700
C1—C2	1.375 (4)	C6—H6B	0.9700
C1—C5	1.383 (4)	C7—C6^{ii}	1.526 (4)
C1—H1A	0.9300	C7—H7A	0.9700
C2—H2A	0.9300	C7—H7B	0.9700
C3—C4	1.368 (4)		
N1^{i}—Co1—N1	113.61 (13)	C3—C4—C5	120.4 (3)
N1^{i}—Co1—Cl1	104.19 (7)	C3—C4—H4A	119.8
N1—Co1—Cl1	104.19 (7)	C5—C4—H4A	119.8
N1^{i}—Co1—Cl2	104.73 (7)	C1—C5—C4	116.5 (3)
N1—Co1—Cl2	104.73 (7)	C1—C5—C6	122.6 (3)
Cl1—Co1—Cl2	125.73 (5)	C4—C5—C6	120.9 (3)
C2—N1—C3	116.5 (3)	C5—C6—C7	111.7 (3)
C2—N1—Co1	121.5 (2)	C5—C6—H6A	109.3
C3—N1—Co1	121.9 (2)	C7—C6—H6A	109.3
C2—C1—C5	120.0 (3)	C5—C6—H6B	109.3
C2—C1—H1A	120.0	C7—C6—H6B	109.3
C5—C1—H1A	120.0	H6A—C6—H6B	107.9
N1—C2—C1	123.4 (3)	C6—C7—C6^{ii}	111.4 (3)
N1—C2—H2A	118.3	C6—C7—H7A	109.3
C1—C2—H2A	118.3	C6^{ii}—C7—H7A	109.3
N1—C3—C4	123.2 (3)	C6—C7—H7B	109.3
N1—C3—H3A	118.4	C6^{ii}—C7—H7B	109.3
C4—C3—H3A	118.4	H7A—C7—H7B	108.0
C5—C6—C7—C6^{ii}	−176.0 (2)		

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

Fig. 1

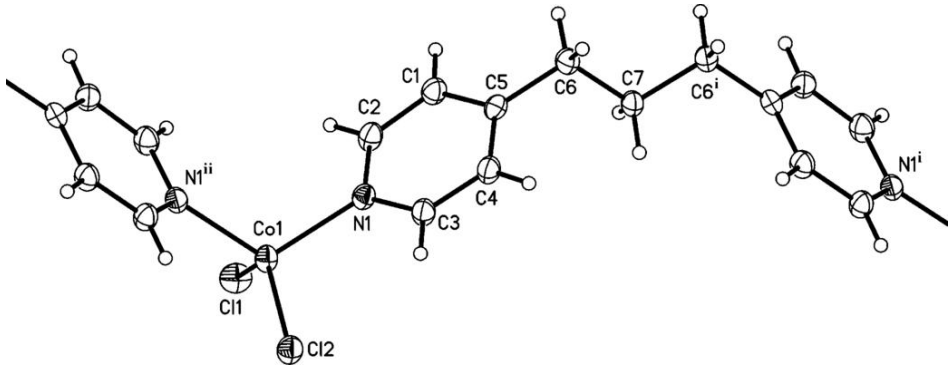

Fig. 2