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

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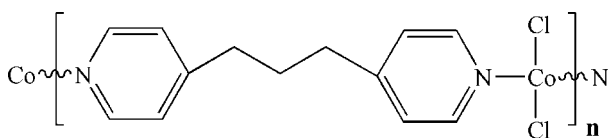
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 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.044; wR factor = 0.099; data-to-parameter ratio = 19.1.

In the title compound, $[\text{CoCl}_2(\text{C}_{13}\text{H}_{14}\text{N}_2)]_n$, 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 bpp ligand is bisected through the central C atom in the chain by a second mirror plane. There are some π - π stacking interactions 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

$[\text{CoCl}_2(\text{C}_{13}\text{H}_{14}\text{N}_2)]_n$
 $M_r = 328.09$
 Monoclinic, $P2_1/m$
 $a = 5.1899$ (10) Å
 $b = 12.989$ (3) Å
 $c = 10.490$ (2) Å
 $\beta = 93.58$ (3)°

$V = 705.8$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.58$ mm⁻¹
 $T = 295$ (2) K
 $0.36 \times 0.25 \times 0.13$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$

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/MSK, 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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supporting information

Acta Cryst. (2008). E64, m1025 [doi:10.1107/S1600536808020862]

catena-Poly[[dichloridocobalt(II)]- μ -1,3-di-4-pyridylpropane- κ^2 N:N']**Wei Xu and Jian-Li Lin****S1. 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)Cl₂]_n (I), obtained by self-assembly from CoCl₂ and bpp in DMF solution. It is isostructural with the previously reported complex [Zn(bpp)Cl₂]_n (Chen, *et al.*, 2004).

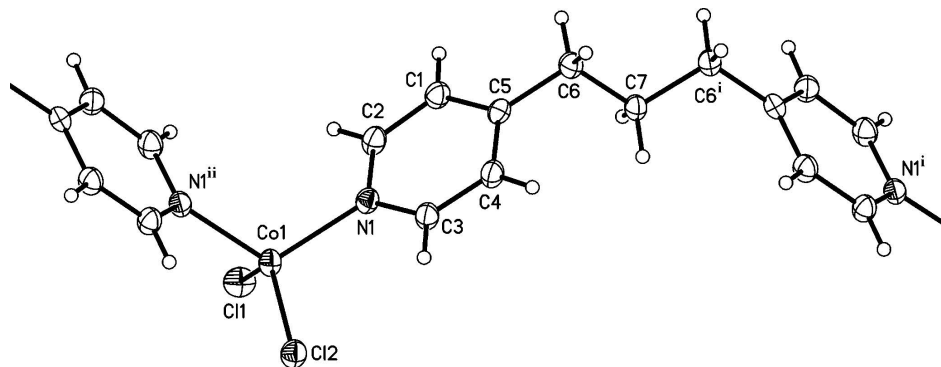
In the title compound, the Co atom is coordinated by two N atoms of two bpp ligands and two Cl anions, forming a distorted tetrahedron (Figure 1 and Table 1.) Both the cation and two chlorine atoms in the coordination polyhedra lie on a mirror plane, while the bpp ligand is bisected through the central 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—C6ⁱ (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 interactions between pyridine rings, which are arranged in a face-to-face fashion with interplanar distances of 3.449 Å.

S2. Experimental

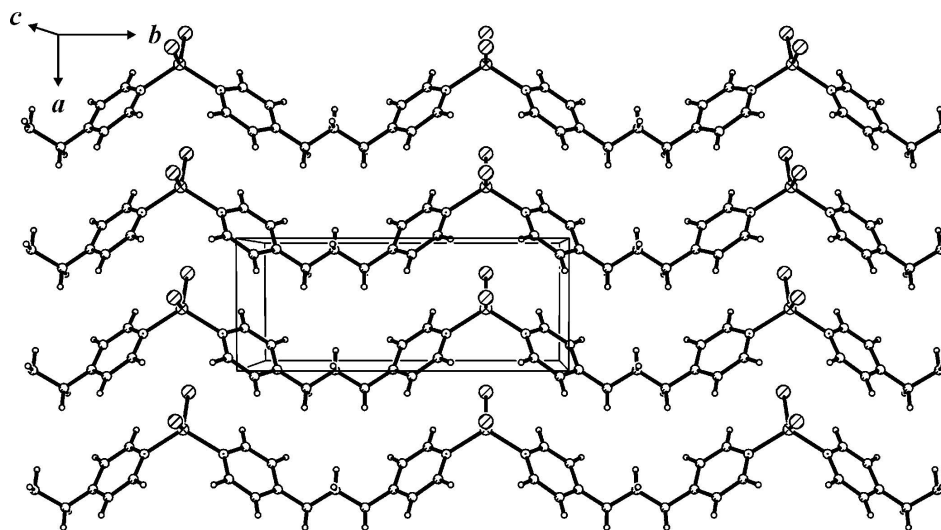
Addition of 1,3-bis(4-pyridyl)propane (bpp) (0.198 g, 1.0 mmol) to a stirred DMF solution (30 ml) of CoCl₂.6H₂O (0.207 g 1.0 mmol) yielded a purple precipitate, which was refluxed for 30 min at 423 K followed by filtration after cooling. The resulting blue filtrate was maintained at room temperature; slow evaporation afforded a small amount of purple platelet crystals 15 days later (yield: 42% based on the initial CoCl₂.6H₂O input).

S3. Refinement

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


Figure 1

ORTEP view of the title compound. The displacement ellipsoids are drawn at 40% probability level.


Figure 2

The crystal packing of the title complex, view parallel to (001).

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

Crystal data

[CoCl₂(C₁₃H₁₄N₂)]

$M_r = 328.09$

Monoclinic, $P2_1/m$

Hall symbol: -P 2yb

$a = 5.1899 (10) \text{ \AA}$

$b = 12.989 (3) \text{ \AA}$

$c = 10.490 (2) \text{ \AA}$

$\beta = 93.58 (3)^\circ$

$V = 705.8 (3) \text{ \AA}^3$

$Z = 2$

$F(000) = 334$

$D_x = 1.544 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4916 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 1.58 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Palte, purple

$0.36 \times 0.25 \times 0.13 \text{ mm}$

Data collection

Rigaku R-AXIS RAPID

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm^{-1}

ω scans

Absorption correction: multi-scan

(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.628$, $T_{\max} = 0.813$

6891 measured reflections

1678 independent reflections

1307 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.057$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$

$h = -6 \rightarrow 6$

$k = -16 \rightarrow 16$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.098$

$S = 1.03$

1678 reflections

88 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.5699P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.56 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.32 \text{ e } \text{\AA}^{-3}$

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 coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| 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 (\AA^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 (\AA , $^\circ$)

| | | | |
|--------------------------|-------------|--------------------------|-----------|
| 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—C6ⁱⁱ -176.0 (2)

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