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***trans*-Bis(aniline- κ N)dichlorobis(ethanol- κ O)cobalt(II)**

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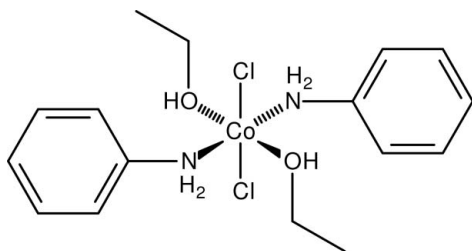
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Key indicators: single-crystal X-ray study; $T = 160$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 13.6.

The title compound, $[\text{CoCl}_2(\text{C}_6\text{H}_7\text{N})_2(\text{C}_2\text{H}_6\text{O})_2]$, was obtained unintentionally as the product of an attempted synthesis of a polycarboxylate-bridged network complex of cobalt(II) using aniline as a base to deprotonate the organic acid. The molecule is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral coordination geometry. Molecules are linked by $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds involving all the potential donors, generating sheets parallel to (001). The phenyl rings protrude on both sides of these sheets and have normal hydrophobic contacts with each other, involving no intercalation or stacking interactions.

Related literature

The corresponding four-coordinate complex without ethanol has tetrahedral geometry (Burrow *et al.*, 1997), with layers of molecules linked by $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds.



Experimental

Crystal data

 $[\text{CoCl}_2(\text{C}_6\text{H}_7\text{N})_2(\text{C}_2\text{H}_6\text{O})_2]$ $M_r = 408.22$ Triclinic, $P\bar{1}$ $a = 5.8166$ (16) Å $b = 6.8339$ (19) Å $c = 12.263$ (3) Å $\alpha = 87.642$ (5)° $\beta = 81.726$ (5)° $\gamma = 73.017$ (5)°
 $V = 461.3$ (2) Å³
 $Z = 1$
Mo $K\alpha$ radiation $\mu = 1.23$ mm⁻¹
 $T = 160$ (2) K
 $0.30 \times 0.20 \times 0.04$ mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)
 $T_{\min} = 0.710$, $T_{\max} = 0.950$ 2296 measured reflections
1583 independent reflections
1278 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.105$
 $S = 1.03$
1583 reflections
116 parametersH atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.82$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.95$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Co—Cl	2.4836 (9)	Co—N	2.175 (3)
Co—O	2.120 (2)		
Cl—Co—O	86.06 (6)	O—Co—N	86.22 (10)
Cl—Co—N	92.33 (8)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}-\text{H1O}\cdots\text{Cl}^{\text{i}}$	0.833 (10)	2.306 (14)	3.114 (2)	163 (3)
$\text{N}-\text{H1C}\cdots\text{Cl}^{\text{ii}}$	0.873 (10)	2.756 (18)	3.560 (3)	154 (3)
$\text{N}-\text{H1D}\cdots\text{Cl}^{\text{i}}$	0.869 (10)	2.574 (13)	3.422 (3)	165 (3)

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

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2117).

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supporting information

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***trans*-Bis(aniline- κ N)dichlorobis(ethanol- κ O)cobalt(II)**

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S1. Comment

The molecule of the title complex, (I) (Fig. 1), is centrosymmetric, so pairs of equivalent ligands lie *trans* to each other in a slightly distorted octahedral coordination geometry, *cis* angles deviating from 90° by less than 4°.

Molecules are linked by O—H...Cl and N—H...Cl hydrogen bonds involving all potential donors, generating sheets parallel to (001), as shown in Fig. 2. The phenyl rings protrude on both sides of these sheets and have normal hydrophobic contacts with each other, involving no intercalation or stacking interactions.

The corresponding four-coordinate complex without ethanol has tetrahedral geometry (Burrow *et al.*, 1997), with layers of molecules linked by N—H...Cl hydrogen bonds.

S2. Experimental

The title compound was obtained unintentionally as the product of an attempted synthesis of a polymeric network complex of cobalt with pyromellitic acid, using vapour diffusion of aniline into an ethanol solution of cobalt(II) chloride and pyromellitic acid at room temperature.

S3. Refinement

H atoms bonded to N and O atoms were located in a difference map and refined with distance restraints of O—H = 0.84 (2) and N—H = 0.87 (2) Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N}, \text{O})$. Other H atoms were positioned geometrically and refined using a riding model (including free rotation about the ethanol C—C bond), with C—H = 0.95–0.99 Å and with $U_{\text{iso}}(\text{H}) = 1.2$ (1.5 for methyl groups) times $U_{\text{eq}}(\text{C})$.

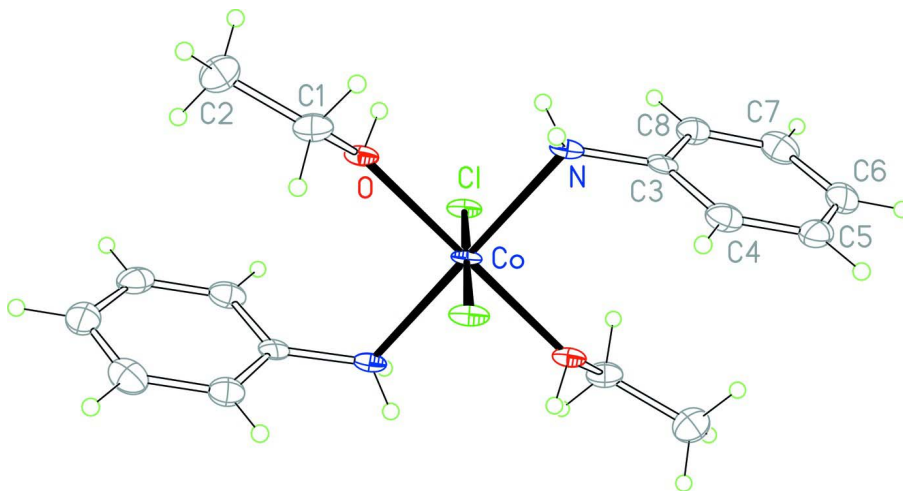


Figure 1

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

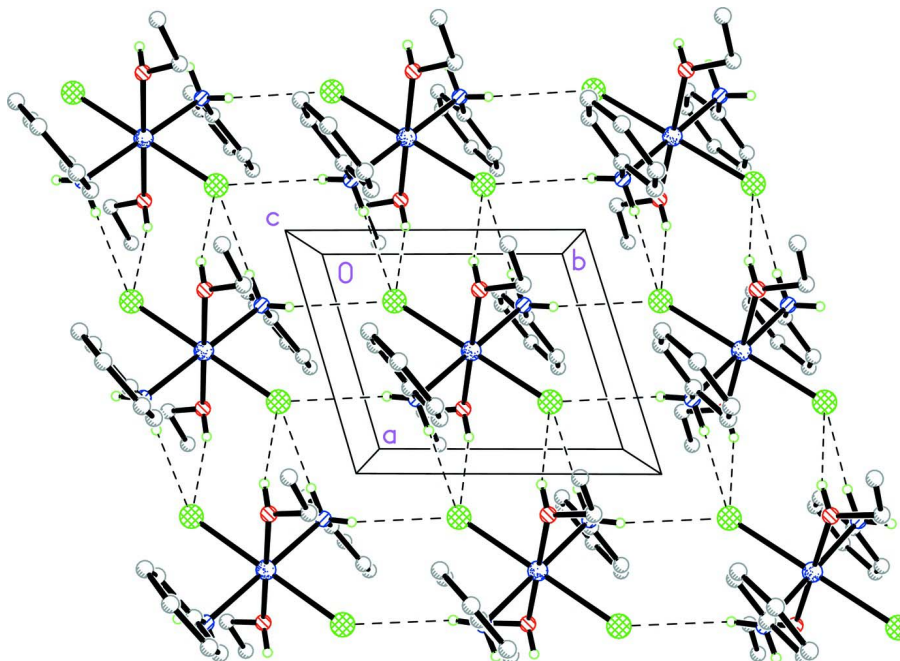


Figure 2

The packing of (I), viewed down the *c* axis, showing one layer of molecules connected by O—H...Cl and N—H...Cl hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

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Crystal data

[CoCl₂(C₆H₇N)₂(C₂H₆O)₂]

M_r = 408.22

Triclinic, *P*1̄

a = 5.8166 (16) Å

b = 6.8339 (19) Å

c = 12.263 (3) Å

α = 87.642 (5)°

β = 81.726 (5)°

γ = 73.017 (5)°

V = 461.3 (2) Å³

Z = 1

F(000) = 213

D_x = 1.469 Mg m⁻³

Mo *K* α radiation, λ = 0.71073 Å

Cell parameters from 2052 reflections

θ = 3.1–28.6°

μ = 1.23 mm⁻¹

T = 160 K

Block, pink

0.30 × 0.20 × 0.04 mm

Data collection

Bruker SMART 1K CCD area-detector
diffractometer

Radiation source: sealed tube

Graphite monochromator

Detector resolution: 8.192 pixels mm⁻¹

thin-slice ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 2004)

T_{min} = 0.710, *T_{max}* = 0.950

2296 measured reflections

1583 independent reflections

1278 reflections with *I* > 2 σ (*I*)

R_{int} = 0.027

θ_{\max} = 25.0°, θ_{\min} = 1.7°

h = -6→6

k = -8→7

l = -14→14

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.105$

$S = 1.03$

1583 reflections

116 parameters

3 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2]$

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

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

$\Delta\rho_{\max} = 0.82 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.95 \text{ e } \text{\AA}^{-3}$

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co	0.5000	0.5000	0.5000	0.0127 (2)
Cl	0.26740 (13)	0.26735 (11)	0.45695 (6)	0.0178 (2)
O	0.2256 (4)	0.5979 (3)	0.63639 (18)	0.0165 (5)
H1O	0.095 (4)	0.608 (5)	0.613 (3)	0.020*
C1	0.2075 (6)	0.7554 (5)	0.7133 (3)	0.0215 (8)
H1A	0.1462	0.8907	0.6787	0.026*
H1B	0.3710	0.7442	0.7319	0.026*
C2	0.0399 (7)	0.7412 (6)	0.8177 (3)	0.0291 (9)
H2A	-0.1218	0.7512	0.7995	0.044*
H2B	0.0287	0.8532	0.8674	0.044*
H2C	0.1041	0.6099	0.8539	0.044*
N	0.2846 (5)	0.7522 (4)	0.4102 (2)	0.0158 (6)
H1C	0.293 (7)	0.860 (3)	0.444 (3)	0.019*
H1D	0.139 (3)	0.743 (5)	0.432 (3)	0.019*
C3	0.3387 (6)	0.7559 (4)	0.2928 (3)	0.0153 (7)
C4	0.5275 (6)	0.8296 (5)	0.2440 (3)	0.0225 (8)
H4	0.6184	0.8803	0.2885	0.027*
C5	0.5829 (7)	0.8292 (5)	0.1308 (3)	0.0267 (8)
H5	0.7112	0.8811	0.0979	0.032*
C6	0.4557 (7)	0.7549 (5)	0.0649 (3)	0.0292 (9)
H6	0.4958	0.7547	-0.0130	0.035*
C7	0.2666 (7)	0.6797 (5)	0.1139 (3)	0.0274 (8)
H7	0.1777	0.6273	0.0692	0.033*
C8	0.2086 (6)	0.6813 (5)	0.2273 (3)	0.0209 (8)
H8	0.0789	0.6311	0.2603	0.025*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0061 (3)	0.0094 (3)	0.0209 (4)	0.0015 (2)	-0.0035 (2)	-0.0010 (2)
Cl	0.0090 (4)	0.0140 (4)	0.0297 (5)	-0.0008 (3)	-0.0050 (3)	-0.0037 (3)
O	0.0090 (12)	0.0161 (11)	0.0240 (13)	-0.0006 (9)	-0.0058 (10)	-0.0030 (9)
C1	0.0161 (18)	0.0168 (17)	0.031 (2)	-0.0030 (14)	-0.0039 (15)	-0.0049 (14)
C2	0.029 (2)	0.0248 (19)	0.031 (2)	-0.0056 (16)	0.0007 (17)	-0.0067 (16)

N	0.0097 (14)	0.0112 (13)	0.0248 (16)	0.0009 (11)	-0.0049 (12)	-0.0015 (11)
C3	0.0124 (17)	0.0069 (14)	0.0227 (17)	0.0036 (12)	-0.0032 (13)	0.0009 (12)
C4	0.0173 (19)	0.0158 (16)	0.035 (2)	-0.0046 (14)	-0.0069 (15)	0.0042 (14)
C5	0.0185 (19)	0.0197 (18)	0.036 (2)	0.0002 (15)	0.0019 (16)	0.0078 (15)
C6	0.030 (2)	0.0197 (18)	0.028 (2)	0.0065 (16)	-0.0001 (16)	0.0035 (15)
C7	0.030 (2)	0.0189 (17)	0.032 (2)	-0.0016 (15)	-0.0120 (16)	-0.0043 (15)
C8	0.0184 (18)	0.0155 (17)	0.0280 (19)	-0.0030 (14)	-0.0042 (14)	-0.0004 (14)

Geometric parameters (Å, °)

Co—Cl	2.4836 (9)	N—H1C	0.873 (10)
Co—Cl ⁱ	2.4835 (9)	N—H1D	0.869 (10)
Co—O	2.120 (2)	N—C3	1.431 (4)
Co—O ⁱ	2.120 (2)	C3—C4	1.388 (5)
Co—N	2.175 (3)	C3—C8	1.382 (5)
Co—N ⁱ	2.175 (3)	C4—H4	0.950
O—H1O	0.833 (10)	C4—C5	1.378 (5)
O—C1	1.431 (4)	C5—H5	0.950
C1—H1A	0.990	C5—C6	1.372 (6)
C1—H1B	0.990	C6—H6	0.950
C1—C2	1.512 (5)	C6—C7	1.396 (6)
C2—H2A	0.980	C7—H7	0.950
C2—H2B	0.980	C7—C8	1.383 (5)
C2—H2C	0.980	C8—H8	0.950
Cl—Co—Cl ⁱ	180	H2A—C2—H2B	109.5
Cl—Co—O	86.06 (6)	H2A—C2—H2C	109.5
Cl ⁱ —Co—O ⁱ	86.06 (7)	H2B—C2—H2C	109.5
Cl ⁱ —Co—O	93.94 (7)	Co—N—H1C	103 (2)
Cl—Co—O ⁱ	93.94 (6)	Co—N—H1D	101 (2)
Cl—Co—N	92.33 (8)	Co—N—C3	118.62 (19)
Cl ⁱ —Co—N	87.67 (8)	H1C—N—H1D	106 (3)
Cl ⁱ —Co—N ⁱ	92.33 (8)	H1C—N—C3	115 (2)
Cl—Co—N ⁱ	87.67 (8)	H1D—N—C3	112 (2)
O—Co—O ⁱ	180	N—C3—C4	119.9 (3)
O—Co—N	86.22 (10)	N—C3—C8	120.5 (3)
O ⁱ —Co—N	93.78 (10)	C4—C3—C8	119.6 (3)
O ⁱ —Co—N ⁱ	86.22 (10)	C3—C4—H4	120.1
O—Co—N ⁱ	93.78 (10)	C3—C4—C5	119.9 (3)
N—Co—N ⁱ	180	H4—C4—C5	120.1
Co—O—H1O	106 (3)	C4—C5—H5	119.5
Co—O—C1	126.4 (2)	C4—C5—C6	121.1 (4)
H1O—O—C1	113 (3)	H5—C5—C6	119.5
O—C1—H1A	109.3	C5—C6—H6	120.4
O—C1—H1B	109.3	C5—C6—C7	119.1 (4)
O—C1—C2	111.8 (3)	H6—C6—C7	120.4
H1A—C1—H1B	107.9	C6—C7—H7	119.9
H1A—C1—C2	109.3	C6—C7—C8	120.1 (3)

H1B—C1—C2	109.3	H7—C7—C8	119.9
C1—C2—H2A	109.5	C3—C8—C7	120.2 (3)
C1—C2—H2B	109.5	C3—C8—H8	119.9
C1—C2—H2C	109.5	C7—C8—H8	119.9
Cl—Co—O—C1	-177.0 (2)	Co—N—C3—C8	96.5 (3)
Cl ⁱ —Co—O—C1	3.0 (2)	N—C3—C4—C5	178.7 (3)
N—Co—O—C1	-84.4 (2)	C8—C3—C4—C5	0.4 (5)
N ⁱ —Co—O—C1	95.6 (2)	C3—C4—C5—C6	-0.6 (5)
Co—O—C1—C2	-162.3 (2)	C4—C5—C6—C7	0.3 (5)
Cl—Co—N—C3	-79.7 (2)	C5—C6—C7—C8	0.3 (5)
Cl ⁱ —Co—N—C3	100.3 (2)	N—C3—C8—C7	-178.1 (3)
O—Co—N—C3	-165.6 (2)	C4—C3—C8—C7	0.2 (5)
O ⁱ —Co—N—C3	14.4 (2)	C6—C7—C8—C3	-0.5 (5)
Co—N—C3—C4	-81.7 (3)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
O—H1O...Cl ⁱⁱ	0.83 (1)	2.31 (1)	3.114 (2)	163 (3)
N—H1C...Cl ⁱⁱⁱ	0.87 (1)	2.76 (2)	3.560 (3)	154 (3)
N—H1D...Cl ⁱⁱ	0.87 (1)	2.57 (1)	3.422 (3)	165 (3)

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