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Poly[[μ_3 -2-(benzotriazol-1-yl)acetato- $\kappa^3 O:O':N^3$]-

chlorido(ethanol-*kO*)cobalt(II)]

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In the title compound, $[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]_n$, the Co^{II} atoms adopt octahedral *trans*-CoN₂O₄ and tetrahedral CoCl₂O₂ coordination geometries (site symmetries $\overline{1}$ and *m*, respectively). The bridging μ_3 -O:O:N 2-(benzotriazol-1-yl)acetato ligands connect the octahedral cobalt nodes into (010) sheets and the CoCl₂ fragments link the sheets into a tri-periodic network. The structure displays O-H···O hydrogen bonding and the ethanol molecule is disordered over two orientations.



Structure description

As a ligand with multiple coordination sites, benzotriazole is a good linker in the generation of metal-organic frameworks (MOFs) as it can bridge different metal cations to afford coordination polymers that exhibit structural diversity and facile accessibility of functionalized new magnetic materials (Bai *et al.*, 2008; Shao *et al.*, 2008; Müller-Buschbaum & Mokaddem, 2006). Functional groups such as carboxylate, hydroxy and pyridyl can be added to the benzotriazole core, increasing its coordination possibilities (Stoumpos *et al.*, 2008; Zhang *et al.*, 2007; Hu *et al.*, 2008; Hang & Ye, 2008). 1*H*-Benzotriazole-1-acetic acid (Hbtaa), a flexible ligand, containing a carboxylate group (when deprotonated) and a triazole unit has been used to construct MOFs (Zheng *et al.*, 2010; Zeng, 2013). As part of our work in this area, we now report the synthesis and crystal structure of the title coordination polymer, $[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]_n$, where $C_8H_6N_3O_2^-$ (L^-) is the 2-benzotriazol-1-yl)acetate anion.

Single-crystal structural analysis reveals that the asymmetric unit consists of two Co^{II} cations (one with site symmetry *m* and one with site symmetry $\overline{1}$), one L^- ligand, two chloride ions (both site symmetry *m*) and one disordered ethanol molecule (Fig. 1). Co1 is four-coordinated by two L^- ligands in O-monodentate mode and two μ^1 -chloride ions in a tetrahedral coordination geometry, whereas Co2 is six-coordinated by four L^- ligands





Figure 1

The asymmetric unit of the title compound showing 50% displacement ellipsoids. Only one orientation of the disordered ethanol molecule is shown.

(two in N-monodentate mode and two in O-monodentate mode) and two ethanol molecules. In the extended structure, the μ^3 -O,O,N bridging L^- ligand links the Co2 nodes into (010) sheets (Fig. 2) and the $Co1Cl_2$ fragments link the sheets into a tri-periodic network (Fig. 3). An O-H···O hydrogen bond (Table 1) occurs.

Synthesis and crystallization

CoCl₂ (1.00 mmol) and 2-(benzotriazol-1-yl) acetic acid (1.00 mmol) were mixed in 10.0 ml of ethanol with stirring for about 30 min at room temperature. Blue block-shaped crystals of the title compound were collected by filtration in 40% yield. Analysis (%) calculated (Found) for C₁₀H₁₂O₃N₃ClCo: C, 37.94 (37.72); H, 3.82 (3.89); N, 13.27 (13.32).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.



Figure 2 Part of a (010) sheet in the title compound.

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
O3−H3···O1	0.86 (1)	2.01 (2)	2.734 (3)	141 (2)

Table 2	
Experimental	details.

Crystal data	
Chemical formula	$[Co(C_8H_6N_3O_2)Cl(C_2H_5OH)]$
$M_{\rm r}$	316.61
Crystal system, space group	Orthorhombic, Pnma
Temperature (K)	223
a, b, c (Å)	9.681 (2), 18.411 (4), 13.163 (3)
$V(Å^3)$	2346.1 (9)
Z	8
Radiation type	Μο Κα
$\mu \text{ (mm}^{-1})$	1.69
Crystal size (mm)	$0.25 \times 0.15 \times 0.09$
Data collection	
Diffractometer	Bruker SMART CCD
Absorption correction	Multi-scan (SADABS; Krause et al., 2015)
T_{\min}, T_{\max}	0.745, 0.859
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	13580, 3058, 2337
R _{int}	0.037
$(\sin \theta / \lambda)_{\max} (\text{\AA}^{-1})$	0.672
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.045, 0.120, 1.09
No. of reflections	3058
No. of parameters	184
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta \rho_{\rm max}, \Delta \rho_{\rm min} \ (e \ {\rm \AA}^{-3})$	0.71, -0.38

Computer programs: SMART and SAINT (Bruker, 2002), SHELXD1997 and SHELXL (Sheldrick, 2008) and OLEX2 (Dolomanov et al., 2009).



Figure 3 The three-dimensional network in the title compound.

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full crystallographic data

IUCrData (2024). **9**, x240630 [https://doi.org/10.1107/S2414314624006308]

Poly[[μ_3 -2-(benzotriazol-1-yl)acetato- $\kappa^3 O:O':N^3$]chlorido(ethanol- κO)cobalt(II)]

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Poly[[μ_3 -2-(benzotriazol-1-yl)acetato- $\kappa^3 O:O':N^3$]chlorido(ethanol- κO)cobalt(II)]

Crystal data	
$[Co(C_8H_6N_3O_2)Cl(C_2H_6O)]$ $M_r = 316.61$ Orthorhombic, <i>Pnma</i> a = 9.681 (2) Å b = 18.411 (4) Å c = 13.163 (3) Å V = 2346.1 (9) Å ³ Z = 8 F(000) = 1288	$D_x = 1.793 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ Å}$ Cell parameters from 39979 reflections $\theta = 2.6-27.6^{\circ}$ $\mu = 1.69 \text{ mm}^{-1}$ T = 223 K Block, blue $0.25 \times 0.15 \times 0.09 \text{ mm}$
Data collection	
Bruker SMART CCD diffractometer ω scans Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015) $T_{\min} = 0.745$, $T_{\max} = 0.859$ 13580 measured reflections	3058 independent reflections 2337 reflections with $I > 2\sigma(I)$ $R_{int} = 0.037$ $\theta_{max} = 28.5^{\circ}, \theta_{min} = 1.9^{\circ}$ $h = -12 \rightarrow 13$ $k = -23 \rightarrow 24$ $l = -11 \rightarrow 17$
Refinement	
Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.045$ $wR(F^2) = 0.120$ S = 1.09 3058 reflections 184 parameters 3 restraints Primary atom site location: dual	Hydrogen site location: mixed H atoms treated by a mixture of independent and constrained refinement $w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 2.3224P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 0.71$ e Å ⁻³ $\Delta\rho_{min} = -0.38$ e Å ⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters $(Å^2)$

	x	у	Ζ	$U_{ m iso}$ */ $U_{ m eq}$	Occ. (<1)
Col	0.43288 (6)	0.2500	0.34271 (4)	0.03019 (17)	

Co2	0.5000	0.5000	0.5000	0.02529 (16)	
Cl1	0.34331 (13)	0.2500	0.18726 (8)	0.0404 (3)	
Cl2	0.27129 (14)	0.2500	0.46492 (10)	0.0472 (3)	
01	0.5318 (2)	0.33968 (11)	0.37700 (15)	0.0296 (4)	
O2	0.5907 (2)	0.45529 (11)	0.36795 (15)	0.0288 (4)	
O3	0.4442 (3)	0.40048 (12)	0.55516 (16)	0.0404 (6)	
Н3	0.448 (4)	0.3656 (8)	0.5120 (12)	0.061*	
N1	0.6491 (2)	0.44636 (13)	0.16425 (17)	0.0279 (5)	
N2	0.7812 (3)	0.44389 (13)	0.13833 (18)	0.0303 (5)	
N3	0.8091 (3)	0.50073 (13)	0.08376 (18)	0.0296 (5)	
C1	0.5701 (3)	0.39542 (15)	0.3296 (2)	0.0245 (6)	
C2	0.4659 (6)	0.3692 (2)	0.6509 (3)	0.0657 (13)	
H2AA	0.4721	0.4093	0.6986	0.079*	0.507 (11)
H2AB	0.3817	0.3432	0.6674	0.079*	0.507 (11)
H2BC	0.5343	0.3314	0.6415	0.079*	0.493 (11)
H2BD	0.5090	0.4063	0.6925	0.079*	0.493 (11)
C3	0.5741 (13)	0.3227 (7)	0.6741 (10)	0.095 (4)	0.507 (11)
H3A	0.6599	0.3487	0.6695	0.143*	0.507 (11)
H3B	0.5747	0.2829	0.6270	0.143*	0.507 (11)
H3C	0.5626	0.3045	0.7419	0.143*	0.507 (11)
C4	0.5894 (3)	0.38538 (16)	0.2171 (2)	0.0303 (6)	
H4A	0.6480	0.3433	0.2062	0.036*	
H4B	0.5002	0.3748	0.1870	0.036*	
C5	0.6926 (3)	0.54205 (16)	0.0755 (2)	0.0297 (6)	
C6	0.5883 (3)	0.50689 (16)	0.1263 (2)	0.0303 (6)	
C7	0.4538 (3)	0.5326 (2)	0.1284 (3)	0.0388 (7)	
H7	0.3835	0.5079	0.1619	0.047*	
C8	0.4311 (4)	0.5955 (2)	0.0789 (3)	0.0464 (9)	
H8	0.3422	0.6146	0.0776	0.056*	
C9	0.5380 (4)	0.6334 (2)	0.0290 (3)	0.0446 (8)	
H9	0.5181	0.6775	-0.0022	0.053*	
C10	0.6678 (4)	0.60771 (17)	0.0254 (2)	0.0389 (7)	
H10	0.7376	0.6324	-0.0087	0.047*	
C3A	0.3657 (10)	0.3405 (5)	0.7065 (6)	0.061 (3)	0.493 (11)
H3AA	0.3169	0.3050	0.6670	0.092*	0.493 (11)
H3AB	0.3030	0.3781	0.7272	0.092*	0.493 (11)
H3AC	0.4047	0.3178	0.7655	0.092*	0.493 (11)

Atomic displacement parameters (\mathring{A}^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Col	0.0432 (4)	0.0220 (3)	0.0254 (3)	0.000	0.0007 (2)	0.000
Co2	0.0336 (3)	0.0231 (3)	0.0191 (3)	-0.0040 (2)	-0.0011 (2)	-0.0030 (2)
Cl1	0.0500(7)	0.0401 (6)	0.0310 (6)	0.000	-0.0062(5)	0.000
Cl2	0.0544 (7)	0.0450 (7)	0.0423 (6)	0.000	0.0154 (6)	0.000
01	0.0409 (11)	0.0250 (10)	0.0230 (10)	-0.0056 (9)	0.0008 (9)	0.0008 (8)
O2	0.0389 (11)	0.0259 (10)	0.0217 (9)	-0.0043 (8)	0.0033 (8)	-0.0050 (8)
O3	0.0704 (16)	0.0263 (11)	0.0245 (11)	-0.0106 (11)	-0.0037 (11)	-0.0014 (9)

N1	0.0327 (12)	0.0291 (12)	0.0220 (11)	-0.0024 (10)	0.0040 (10)	0.0015 (9)
N2	0.0369 (13)	0.0287 (12)	0.0252 (12)	0.0001 (11)	0.0060 (10)	0.0035 (10)
N3	0.0351 (13)	0.0273 (12)	0.0265 (12)	-0.0005 (10)	0.0046 (11)	0.0059 (10)
C1	0.0249 (13)	0.0263 (14)	0.0223 (13)	0.0001 (11)	-0.0018 (11)	0.0015 (10)
C2	0.112 (4)	0.047 (2)	0.038 (2)	-0.001 (2)	-0.014 (2)	0.0075 (18)
C3	0.111 (10)	0.079 (8)	0.096 (9)	0.013 (7)	-0.004 (7)	0.027 (6)
C4	0.0430 (16)	0.0242 (13)	0.0238 (13)	-0.0065 (12)	0.0059 (12)	-0.0004 (11)
C5	0.0386 (16)	0.0295 (14)	0.0210 (13)	-0.0006 (12)	0.0021 (12)	0.0013 (11)
C6	0.0385 (15)	0.0307 (15)	0.0217 (13)	0.0012 (12)	0.0007 (12)	-0.0015 (11)
C7	0.0369 (16)	0.0463 (19)	0.0332 (17)	0.0021 (15)	0.0027 (14)	-0.0039 (15)
C8	0.047 (2)	0.054 (2)	0.0388 (19)	0.0146 (17)	-0.0046 (16)	-0.0047 (16)
C9	0.062 (2)	0.0367 (18)	0.0351 (18)	0.0117 (16)	-0.0053 (16)	0.0043 (15)
C10	0.055 (2)	0.0334 (16)	0.0281 (15)	0.0023 (15)	0.0004 (15)	0.0046 (13)
C3A	0.082 (6)	0.069 (6)	0.033 (4)	-0.019 (5)	0.003 (4)	0.007 (4)

Geometric parameters (Å, °)

Co1—Cl1	2.2223 (13)	C2—H2BC	0.9700	
Co1—Cl2	2.2439 (14)	C2—H2BD	0.9700	
Co1-O1 ⁱ	1.961 (2)	C2—C3	1.387 (12)	
Co101	1.961 (2)	C2—C3A	1.324 (9)	
Co2—O2	2.114 (2)	С3—НЗА	0.9600	
Co2—O2 ⁱⁱ	2.114 (2)	С3—Н3В	0.9600	
Co2—O3 ⁱⁱ	2.043 (2)	С3—НЗС	0.9600	
Co2—O3	2.043 (2)	C4—H4A	0.9700	
Co2—N3 ⁱⁱⁱ	2.152 (3)	C4—H4B	0.9700	
Co2—N3 ^{iv}	2.152 (3)	C5—C6	1.373 (4)	
01—C1	1.257 (3)	C5—C10	1.397 (4)	
O2—C1	1.228 (3)	C6—C7	1.386 (5)	
O3—H3	0.859 (9)	С7—Н7	0.9300	
O3—C2	1.401 (4)	C7—C8	1.347 (5)	
N1—N2	1.324 (3)	C8—H8	0.9300	
N1C4	1.441 (4)	C8—C9	1.410 (5)	
N1-C6	1.356 (4)	С9—Н9	0.9300	
N2—N3	1.298 (3)	C9—C10	1.344 (5)	
N3—Co2 ^v	2.152 (2)	C10—H10	0.9300	
N3—C5	1.365 (4)	СЗА—НЗАА	0.9600	
C1—C4	1.505 (4)	СЗА—НЗАВ	0.9600	
C2—H2AA	0.9700	СЗА—НЗАС	0.9600	
C2—H2AB	0.9700			
Cl1—Co1—Cl2	112.83 (6)	C3—C2—O3	124.4 (7)	
O1—Co1—Cl1	113.73 (6)	C3—C2—H2AA	106.2	
Ol ⁱ —Col—Cll	113.73 (6)	C3—C2—H2AB	106.2	
O1—Co1—Cl2	100.10 (7)	C3A—C2—O3	123.4 (6)	
Ol ⁱ —Col—Cl2	100.10 (7)	C3A—C2—H2BC	106.5	
01-C01-01 ⁱ	114.66 (13)	C3A—C2—H2BD	106.5	
O2 ⁱⁱ —Co2—O2	180.0	С2—С3—НЗА	109.5	

O2 ⁱⁱ —Co2—N3 ⁱⁱⁱ	93.56 (9)	C2—C3—H3B	109.5
O2—Co2—N3 ⁱⁱⁱ	86.44 (9)	C2—C3—H3C	109.5
O2 ⁱⁱ —Co2—N3 ^{iv}	86.44 (9)	H3A—C3—H3B	109.5
O2—Co2—N3 ^{iv}	93.56 (9)	H3A—C3—H3C	109.5
O3—Co2—O2	93.03 (8)	H3B—C3—H3C	109.5
O3 ⁱⁱ —Co2—O2 ⁱⁱ	93.03 (8)	N1—C4—C1	115.4 (2)
O3 ⁱⁱ —Co2—O2	86.97 (8)	N1—C4—H4A	108.4
O3—Co2—O2 ⁱⁱ	86.97 (8)	N1—C4—H4B	108.4
O3 ⁱⁱ —Co2—O3	180.0	C1—C4—H4A	108.4
Q3—Co2—N3 ⁱⁱⁱ	87.74 (10)	C1—C4—H4B	108.4
$O3-Co2-N3^{iv}$	92.26 (10)	H4A—C4—H4B	107.5
$O3^{ii}$ — $Co2$ — $N3^{iii}$	92.25 (10)	N3-C5-C6	107.8 (2)
$O3^{ii}$ — $Co2$ — $N3^{iv}$	87 75 (10)	N_{3} C5 C10	1314(3)
$N3^{iii}$ —Co2—N3 ^{iv}	180.0	C6-C5-C10	120.8(3)
$C_1 = 0_1 = C_0_1$	135.83 (19)	N1 - C6 - C5	1044(3)
$C_1 = 0^2 = C_0^2$	128 27 (18)	N1 - C6 - C7	1330(3)
$C_{0}^{2} = 0^{3} = H^{3}$	120.27(10) 1150(14)	C_{5}	122.6(3)
$C_{2}^{2} = 0^{3} = C_{0}^{2}$	113.0(14) 130.4(2)	C6-C7-H7	122.0(3)
$C_2 = 03 = 002$	106.3(14)	$C_{0} = C_{1} = C_{0}$	122.0 115.9(3)
$N_2 - N_1 - C_4$	100.3(14) 119.0(2)	C8-C7-H7	122.0
$N_2 = N_1 = C_4$	119.0(2) 110.6(2)	C7 - C8 - H8	119.0
C6-N1-C4	130.1(3)	C7 - C8 - C9	119.0 122.1(3)
N3_N2_N1	108.4(2)	C9-C8-H8	119.0
$N_2 = N_3 = C_0 2^{v}$	100.4(2) 117 20 (19)	C8-C9-H9	119.0
$N_2 = N_3 = C_0 Z$	108.8(2)	C_{10} C_{9} C_{8}	119.0 121.9(3)
112 - 113 - C3 C5 - 113 - Co2 ^v	100.0(2) 132 23 (19)	$C_{10} - C_{9} - C_{8}$	121.9 (3)
$C_{1} - C_{1} - C_{4}$	152.25(17)	$C_{10} - C_{10} - H_{10}$	121.7
$0^{2}-0^{1}-0^{1}$	115.1(2) 125.2(3)	C9-C10-C5	121.7 116.6(3)
$0^{2}-C^{1}-C^{4}$	129.2(3)	C9-C10-H10	121 7
$O_2 - C_1 - C_7$ $O_3 - C_2 - H_2 \Delta \Delta$	106.2	$C_2 = C_3 \Delta = H_3 \Delta \Delta$	109.5
$O_3 - C_2 - H_2 AB$	106.2	$C_2 = C_3 A = H_3 A B$	109.5
$O_3 - C_2 - H_2BC$	106.5	$C_2 = C_3 A = H_3 A C$	109.5
$O_3 - C_2 - H_2 BD$	106.5	$H_{3} = C_{3} = H_{3} = H_{3$	109.5
$H_{2AA} = H_{2AB}$	106.5	$H_{3AA} = C_{3A} = H_{3AC}$	109.5
$H_{2}R_{2} = H_{2}R_{2}$	106.5	$H_{3AB} = C_{3A} = H_{3AC}$	109.5
11200 02 11200	100.5	HIMD CIN HIMC	109.5
$C_{01} - 01 - C_{1} - 02$	154.9(2)	N2—N3—C5—C10	-1799(3)
$C_{01} - 0_{1} - C_{1} - C_{4}$	-24.5(2)	N_{3} C5 C6 N_{1}	11(3)
$C_{0}^{2} = 0^{2} = 0^{2} = 0^{1} = 0^{1}$	-27.3(4)	N_{3} C_{5} C_{6} C_{7}	-1767(3)
$C_{02} = 02 = C_1 = C_4$	1521(2)	$N_3 = C_5 = C_1 0 = C_9$	170.7(3)
$C_{02} = 02 = 01 = 04$	-96.0(8)	C4 N1 N2 N3	177.7(3) 174.0(2)
$C_{02} = 03 = 02 = 03$	127.9 (6)	C4 N1 $C6$ $C5$	-174.1(3)
$C_{02}^{v} = N_{3}^{v} = C_{5}^{v} = C_{6}^{v}$	127.5(0) 162.5(2)	C4 - N1 - C6 - C7	33(5)
$C_{02}^{v} = N_{3} = C_{5} = C_{10}^{v}$	-160(5)	$C_{1} = C_{1} = C_{1$	-1.3(5)
01 - C1 - C4 - N1	$-172 \ 8 \ (3)$	C_{6} N1 N2 N3	-0.5(3)
02-C1-C4-N1	7 8 (4)	C6-N1-C4-C1	-843(4)
$N1 - N2 - N3 - Co2^{v}$	-165 54 (18)	C_{6} C_{5} C_{10} C_{9}	-0.7(5)
N1—N2—N3—C5	11(3)	C6 - C7 - C8 - C9	-0.8(5)
111 112 113 -03	1.1 (3)	000100000	0.0 (5)

data reports

N1—C6—C7—C8	-178.3 (3)	C7—C8—C9—C10	2.1 (6)
N2—N1—C4—C1	102.4 (3)	C8—C9—C10—C5	-1.3 (5)
N2—N1—C6—C5	-0.4 (3)	C10-C5-C6-N1	179.8 (3)
N2—N1—C6—C7	177.0 (3)	C10-C5-C6-C7	2.0 (5)
N2—N3—C5—C6	-1.4 (3)		

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

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	<i>D</i> —H··· <i>A</i>
O3—H3…O1	0.86 (1)	2.01 (2)	2.734 (3)	141 (2)