catena-Poly[{μ 3 -3,3′-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methyl)]]}

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The title compound, \([\text{Co(C}_{24}\text{H}_{28}\text{N}_{2}\text{O}_{6})]_n\), crystallizes as infinite chains related to one another by inversion centers, giving a centrosymmetric coordination polymer. The Co\(II\) ion, situated on a twofold rotation axis, forms a complex with the crown-4 moiety of the 3,3'-(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)dibenzoate anion. The distorted octahedral coordination sphere of the Co\(II\) ion is completed by two carboxylate O atoms from two bridging intra-chain ligands. Metallomacrocyclic rings of 16 atoms are present, with each ring containing two Co\(II\) ions and 14 atoms from the bridging ligands. These units repeat as infinite zigzag chains along [101].

**Related literature**

For the structures of coordination polymers (CPs) or compounds with metal-organic frameworks including one-dimensional CPs or MOFs, see: Du \textit{et al.} (2013); Ingram \textit{et al.} (2012, 2013); Janiak (2013); Leong & Vittal (2011).

**Experimental**

**Crystal data**

\[
\text{[Co(C}_{24}\text{H}_{28}\text{N}_{2}\text{O}_{6})]}
\]

- \(M_r = 499.41\)
- Monoclinic, \(C2/c\)
- \(a = 20.626\ (2)\ \text{Å}\)
- \(b = 8.9778\ (10)\ \text{Å}\)
- \(c = 13.9263\ (16)\ \text{Å}\)
- \(\beta = 127.051\ (1)\)
- \(V = 2058.2\ (4)\ \text{Å}^3\)
- \(Z = 4\)
- Mo \(K\alpha\) radiation
- \(\mu = 0.88\ \text{mm}^{-1}\)
- \(T = 173\ \text{K}\)
- \(0.40 \times 0.14 \times 0.14\ \text{mm}^3\)

**Data collection**

- Bruker APEXII CCD diffractometer
- Absorption correction: multi-scan (\textit{SADABS}; Bruker, 2012)
- \(T_{\text{min}} = 0.606, T_{\text{max}} = 0.746\)
- 3614 measured reflections
- 2930 independent reflections
- 2290 reflections with \(I > 2\sigma(I)\)
- \(R_{\text{int}} = 0.018\)

**Refinement**

- \(R[F^2 > 2\sigma(F^2)] = 0.049\)
- \(wR(F^2) = 0.125\)
- \(S = 1.02\)
- 2930 reflections
- 150 parameters
- H-atom parameters constrained
- \(\Delta\rho_{\text{max}} = 0.80\ \text{e} \ \text{Å}^{-3}\)
- \(\Delta\rho_{\text{min}} = -0.47\ \text{e} \ \text{Å}^{-3}\)

**Data collection: APEX2** (Bruker, 2011); cell refinement: \textit{SAINT} (Bruker, 2009); data reduction: \textit{SAINT}; program(s) used to solve structure: \textit{SHELXS97} (Sheldrick, 2008); program(s) used to refine structure: \textit{SHELXL97} (Sheldrick, 2008); molecular graphics: \textit{OLEX2} (Dolomanov \textit{et al.}, 2009); software used to prepare material for publication: \textit{OLEX2}.

Financial support of NSF/CREST/ CFNM (award No. HRD-1137751) is acknowledged.

**Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2131).**

**References**

supplementary materials


catena-Poly[(μ₃-3,3’-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)]dibenzoato)cobalt(II)]

Liang Liao, Conrad W. Ingram, John Bacsa and Cass Parker

1. Comment

The title compound is one of a series of coordination polymers prepared from the anionic ligand LH₂, 3,3’-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)]dibenzoate. This ligand shows unusual adaptability in that it displays two complexation modes on binding to metals. The ligand attaches to the metal via two oxygen and two nitrogen atoms (forming a crown complex). The crown forms four bonds to the metal, while an ideal coordination number for a Co²⁺ ion is 6. Thus vacant coordination sites suitable for coordination by the carboxylate groups exist. The carboxylate ions behave as monodentate bridging ligands and the entire ligand is hexadentate. The Co²⁺ atom is moved out of the best plane of the crown since this arrangement is better for forming optimal bonds to the ligand. This new compound is novel in that, although the ligands bridge the metal atoms forming one-dimensional chains, the metal atoms are positioned in the center of the organic linker. Topologically, the Co²⁺ atoms and the ligands forms nodes in the network rather than the metal atoms only.

The title compound is synthesized from the ligand LH₂, 3,3’-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)] dibenzoic acid. The metal atoms are positioned in the center of the organic linker. The asymmetric unit of the compound contains a Co²⁺ ion and deprotonated ligand L with formula C₂₄H₂₈N₂O₆Co. The Co²⁺ ion is 6-coordinate in a distorted octahedral geometry being bound to two N atoms and two O atoms of the crown (1,7-diaza-12-crown-4) and two carboxylic O atoms, one from each of two additional intra-chain ligands (Figure 1s). The Co₁—O₁, Co₁—O₃ and Co₁—N₁ bond lengths are 1.9886 (16), 2.2399 (16) and 2.2213 (17) Å, respectively. The O₁—Co₁—O₁ angle is 104.15 (9)°. The shortest distance between two neighboring Co²⁺ ions along a chain is 9.046 (1) Å. The Co²⁺ ion of the Co(crown-4)²⁺ unit is located on a 2-fold rotation axis. The symmetry independent atoms consist of one half of the ligand with the rotation axis generating the second half of the ligand at the Co atom. Bond circuits consisting of sixteen-membered metallamacrocyle rings can be identified in the structure. Each ring contains two Co²⁺ ions and fourteen non-H atoms of the ligand. Each Co²⁺ ion is a node for three ligands and two connected macrocycle rings. The pair of benzene moieties within a metallamacrocycle ring are remarkably co-planar (the two rings are in the same plane within experimental error). The dihedral angle between this plane and the plane of the next two nearest phenyl rings along the 1-D chain is 68.79 (5)°. Repetition of these units creates a 1-D polymer network with an infinite number of these rings.

2. Experimental

The title compound was synthesized in an autoclave by mixing the ligand, 3,3’-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)]dibenzoic acid, L₇H₇ (4x10⁻⁵ mol), (Ingram et al. (2012), (2013)) Co(NO₃)₂·6H₂O (1.2x10⁻⁴ mol, 35.8 mg), H₂O (12 ml) and pyridine (4x10⁻² ml). The mixture was heated at 130 °C in an autoclave for 7 days and then cooled to ambient temperature. Red crystals were collected and washed with H₂O by filtration. Elem. anal. calcd. C₂₄H₂₈N₂O₆Co %: C, 57.72; H, 5.65; N, 5.61; Found: C, 57.79; H, 5.74; N, 5.46.
3. Refinement

Refinement Refinement of F2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F2, conventional R-factors R are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2σ(F2) is used only for calculating R-factors(gt), etc. and is not relevant to the choice of reflections for refinement. R-factors based on F2 are statistically about twice as large as those based on F and R-factors based on ALL data will be even larger. Computing details Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT (Bruker, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov et al., 2009); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009).

Computing details

Data collection: APEX2 (Bruker, 2011); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT (Bruker, 2009); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: OLEX2 (Dolomanov et al., 2009); software used to prepare material for publication: OLEX2 (Dolomanov et al., 2009).

Figure 1

A view of a portion of one of the chains of (I). Non-H atoms are represented by ellipsoids at the 50% probability level. Sixteen membered metallomacrocycle rings can be identified from this figure.

catena-Poly[[μ3-3,3′-[(1,7-dioxa-4,10-diazacyclododecane-4,10-diyl)bis(methylene)]dibenzoato]cobalt(II)]

Crystal data

[Co(C24H28N2O6)]

F(000) = 1044
Dx = 1.612 Mg m−3

Monoclinic, C2/c

Mo Kα radiation, λ = 0.71073 Å

Cell parameters from 4901 reflections

θ = 2.5–31.0°

μ = 0.88 mm−1

T = 173 K

Needle, red

0.40 × 0.14 × 0.14 mm

Data collection

Bruker D8

diffractometer with a APEXII detector

ω scans with a narrow frame width

Radiation source: fine-focus sealed tube

Absorption correction: multi-scan

Graphite monochromator

(SADABS; Bruker, 2012)

Detector resolution: 512 pixels mm−1

3614 measured reflections

Acta Cryst. (2014). E70, m24
supplementary materials

2930 independent reflections                  h = −28→18
2290 reflections with I > 2σ(I)             k = −12→4
R_{int} = 0.018                                l = −20→19
θ_max = 31.2°, θ_min = 2.6°

Refinement

Refinement on F^2                           Secondary atom site location: difference Fourier map
Least-squares matrix: full                Hydrogen site location: difference Fourier map
R[F^2 > 2σ(F^2)] = 0.049                   H-atom parameters constrained
wR(F^2) = 0.125                           \( w = \frac{1}{\sigma^2(F_0^2) + (0.073P)^2} \)
S = 1.02                               where \( P = (F_0^2 + 2F_c^2)/3 \)
2930 reflections                         (Δ/σ)_{max} < 0.001
150 parameters                           \( \Delta \rho_{\text{max}} = 0.80 \text{ e Å}^{-3} \)
0 restraints                                  \( \Delta \rho_{\text{min}} = -0.47 \text{ e Å}^{-3} \)
Primary atom site location: iterative

Special details

Experimental. Absorption correction: SADABS-2012/1 (Bruker,2012) was used for absorption correction. wR2(int) was
0.0566 before and 0.0407 after correction. The Ratio of minimum to maximum transmission is 0.8118. The λ/2 correction
factor is 0.0015.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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Acta Cryst. (2014). E70, m24
**supplementary materials**

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**Atomic displacement parameters (Å²)**

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**Geometric parameters (Å, °)**

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*Acta Cryst. (2014). E70, m24*
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Symmetry codes: (i) −x+1, y, −z+3/2; (ii) −x+1/2, −y−1/2, −z+1; (iii) x−1/2, −y−1/2, z−1/2; (iv) −x, y, −z+1/2.