

catena-Poly[[triaquacobalt(II)]- μ -5-hydroxybenzene-1,3-dicarboxylato- κ O¹:O³]

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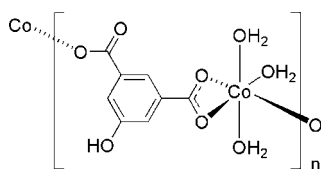
Received 30 September 2007; accepted 8 October 2007

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.051; wR factor = 0.111; data-to-parameter ratio = 13.0.

Crystals of the title compound, $[\text{Co}(\text{C}_8\text{H}_4\text{O}_5)(\text{H}_2\text{O})_3]_n$, were obtained by hydrothermal methods. Each Co^{II} ion is six-coordinated by two O atoms from one 5-hydroxybenzene-1,3-dicarboxylate (L) ligand, one O atom from another L ligand and three water molecules [$\text{Co}-\text{O} = 2.016$ (3)– 2.324 (3) Å]. Each ligand L , acting in a tridentate mode, bridges two Co ions, resulting in the formation of polymeric zigzag chains extending along the [110] direction. The crystal packing is stabilized by an extensive network of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For applications of metal carboxylate coordination polymers in functional materials, see: Cao *et al.* (2004); Chui *et al.* (1999); Lo *et al.* (2000); For low-dimensional coordination polymers extending to high-dimensional networks *via* intermolecular forces, see: Ghoshal *et al.* (2003); Wang *et al.* (2006); Holliday & Mirkin (2001).



Experimental

Crystal data

$[\text{Co}(\text{C}_8\text{H}_4\text{O}_5)(\text{H}_2\text{O})_3]$
 $M_r = 293.09$
Orthorhombic, $Pccn$
 $a = 18.102$ (4) Å
 $b = 7.4538$ (19) Å
 $c = 15.089$ (4) Å

$V = 2035.9$ (9) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 1.72$ mm⁻¹
 $T = 293$ (2) K
 $0.31 \times 0.30 \times 0.25$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.61$, $T_{\text{max}} = 0.71$
(expected range = 0.559–0.651)

10142 measured reflections
2005 independent reflections
1494 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.111$
 $S = 1.03$
2005 reflections

154 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.45$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.58$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O5}-\text{H9}\cdots\text{O3}^{\text{i}}$ | 0.82 | 1.84 | 2.651 (4) | 172 |
| $\text{O6}-\text{H1}\cdots\text{O5}^{\text{ii}}$ | 0.86 | 1.86 | 2.720 (4) | 174 |
| $\text{O6}-\text{H2}\cdots\text{O2}^{\text{iii}}$ | 0.82 | 1.85 | 2.655 (4) | 166 |
| $\text{O7}-\text{H5}\cdots\text{O8}^{\text{iv}}$ | 0.89 | 1.89 | 2.773 (4) | 173 |
| $\text{O7}-\text{H6}\cdots\text{O6}^{\text{v}}$ | 0.82 | 2.17 | 2.913 (4) | 151 |
| $\text{O8}-\text{H3}\cdots\text{O2}^{\text{vi}}$ | 0.88 | 1.74 | 2.612 (4) | 170 |
| $\text{O8}-\text{H4}\cdots\text{O4}^{\text{vii}}$ | 0.82 | 1.86 | 2.634 (4) | 158 |

Symmetry codes: (i) $-x + \frac{3}{2}, y, z - \frac{1}{2}$; (ii) $x + \frac{1}{2}, -y + 1, -z + \frac{1}{2}$; (iii) $-x + 2, -y + 1, -z + 1$; (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (v) $-x + 2, y - \frac{1}{2}, -z + \frac{1}{2}$; (vi) $-x + 2, -y, -z + 1$; (vii) $-x + \frac{3}{2}, -y + \frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2314).

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supplementary materials

Acta Cryst. (2007). E63, m2721 [doi:10.1107/S1600536807049288]

***catena*-Poly[[triaquacobalt(II)]- μ -5-hydroxybenzene-1,3-dicarboxylato- $\kappa O^1:O^3$]**

Y.-H. Hu, Y.-Z. Li, R.-L. Zhang and J.-Y. Wu

Comment

The design and synthesis of supramolecular architectures based on Metal carboxylate coordination polymer networks has been a field of rapid growth recently due to their fascinating architectures and potential applications in functional materials (Cao *et al.*, 2004; Chui *et al.*, 1999; Lo *et al.*, 2000). It is known that low dimensional coordination polymers can extend to high dimensional networks *via* noncovalent intermolecular forces such as hydrogen-bonding and π - π stacking interactions (Ghoshal *et al.*, 2003; Wang *et al.*, 2006; Holliday & Mirkin, 2001.) In this paper, we present the crystal structure of the title compound (I), obtained by hydrothermal reaction of 5-hydroxyisophthalic acid (H₂L) with cobalt acetate. The phenol hydroxy group in the ligand *L* in (I) remains protonated.

In the title compound, [Co(C₈H₄O₅)(H₂O)₃]_n, Co^{II} ion is hexacoordinated in a distorted octahedral geometry by three O atoms from two *L* ligands and three water molecules (Fig. 1). The bond lengths Co1—O1, Co1—O3B, Co1—O4B and Co1—O7 are 2.016 (3) Å, 2.324 (3) Å, 2.076 (3) Å and 2.044 (3) Å, respectively. Atoms O6 and O8 occupy the axial positions with bond lengths Co1—O6 and Co1—O8 of 2.095 (3) and 2.112 (3) Å, respectively [O6—Co1—O8 172.91 (10)°]. Each ligand *L* acting in a tridentate mode bridges two Co ions, that results in formation of polymeric zigzag chains extended along the direction [110] (Fig. 2). The crystal packing is stabilized by extensive network of O—H...O hydrogen bonds (Table 1, Fig. 3).

Experimental

All manipulations were carried out in air. A mixture of Co(OAc)₂·6H₂O (92 mg, 0.5 mmol), Et₃N (54 mg, 0.53 mmol), H₃hdpa (92 mg, 0.5 mmol) and water (10 cm³) were sealed in 23 cm³ Teflon-lined stainless steel parr bomb. The bomb was heated to 393 K for 4 d. Then it was cooled to room temperature to yield amaranthine sheet crystals. Yield: 99 mg (68%).

Refinement

All H atoms were geometrically positioned (C—H 0.93 Å, O—H 0.82–0.89 Å), and refined as riding, with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C}, \text{O})$.

Figures

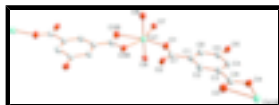


Fig. 1. The *ORTEP* representation of the structure of the title compound showing the atomic numbering and 50% probability displacement ellipsoids [symmetry codes: (A) $-1/2 + x, 1/2 + y, 1 - z$; (B) $1/2 + x, -1/2 + y, 1 - z$]. H atoms omitted for clarity.

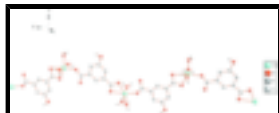


Fig. 2. A portion of polymeric zigzag chain in (I). C-bound H atoms omitted for clarity.

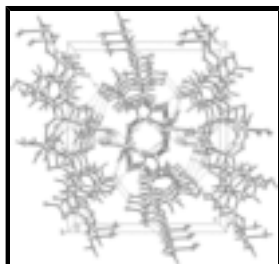


Fig. 3. A packing diagram viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

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Crystal data

[Co(C₈H₄O₅)(H₂O)₃]

M_r = 293.09

Orthorhombic, *Pccn*

Hall symbol: -P 2ab 2ac

a = 18.102 (4) Å

b = 7.4538 (19) Å

c = 15.089 (4) Å

V = 2035.9 (9) Å³

Z = 8

*F*₀₀₀ = 1192

D_x = 1.912 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 882 reflections

θ = 3.8–27.8°

μ = 1.72 mm⁻¹

T = 293 (2) K

Clear, amaranthine

0.31 × 0.30 × 0.25 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293(2) K

ϕ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.61, *T_{max}* = 0.71

10142 measured reflections

2005 independent reflections

1494 reflections with *I* > 2σ(*I*)

R_{int} = 0.061

θ_{\max} = 26.0°

θ_{\min} = 2.3°

h = -22→22

k = -5→9

l = -16→18

Refinement

Refinement on *F*²

Least-squares matrix: full

R [*F*² > 2σ(*F*²)] = 0.051

wR(*F*²) = 0.111

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 1.22P]$

| | |
|--|--|
| $S = 1.03$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2005 reflections | $(\Delta/\sigma)_{\max} < 0.001$ |
| 154 parameters | $\Delta\rho_{\max} = 0.45 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$ |
| | 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|-------------|--------------|----------------------------------|
| Co1 | 1.04346 (3) | 0.17886 (7) | 0.37080 (4) | 0.03052 (19) |
| O1 | 0.94108 (15) | 0.2810 (4) | 0.38571 (18) | 0.0338 (7) |
| O2 | 0.91508 (16) | 0.3204 (4) | 0.52828 (18) | 0.0359 (7) |
| O3 | 0.66360 (16) | 0.5739 (4) | 0.61282 (18) | 0.0362 (7) |
| O4 | 0.59267 (16) | 0.6600 (4) | 0.50529 (18) | 0.0322 (7) |
| O5 | 0.72308 (15) | 0.5429 (3) | 0.22300 (18) | 0.0328 (6) |
| H9 | 0.7601 | 0.5456 | 0.1917 | 0.039* |
| O6 | 1.08354 (15) | 0.4366 (4) | 0.34307 (17) | 0.0300 (6) |
| H1 | 1.1266 | 0.4413 | 0.3183 | 0.036* |
| H2 | 1.0836 | 0.4966 | 0.3886 | 0.036* |
| O7 | 1.03489 (15) | 0.1460 (4) | 0.23670 (19) | 0.0341 (7) |
| H5 | 1.0238 | 0.2373 | 0.2012 | 0.041* |
| H6 | 1.0084 | 0.0595 | 0.2259 | 0.041* |
| O8 | 1.00636 (15) | -0.0888 (4) | 0.38236 (17) | 0.0316 (6) |
| H3 | 1.0374 | -0.1590 | 0.4108 | 0.038* |
| H4 | 0.9690 | -0.0914 | 0.4131 | 0.038* |
| C1 | 0.8272 (2) | 0.4173 (5) | 0.4220 (3) | 0.0287 (9) |
| C2 | 0.7768 (2) | 0.4667 (5) | 0.4871 (3) | 0.0313 (9) |
| H7 | 0.7881 | 0.4493 | 0.5466 | 0.038* |
| C3 | 0.7096 (2) | 0.5416 (5) | 0.4635 (3) | 0.0295 (9) |
| C4 | 0.6928 (2) | 0.5694 (5) | 0.3739 (3) | 0.0271 (8) |
| H8 | 0.6483 | 0.6223 | 0.3576 | 0.032* |
| C5 | 0.7433 (2) | 0.5179 (5) | 0.3099 (3) | 0.0289 (9) |
| C6 | 0.8096 (2) | 0.4427 (6) | 0.3326 (3) | 0.0350 (10) |
| H10A | 0.8429 | 0.4080 | 0.2889 | 0.042* |
| C7 | 0.9002 (2) | 0.3346 (5) | 0.4477 (3) | 0.0298 (9) |

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C8 0.6541 (2) 0.5946 (6) 0.5305 (3) 0.0323 (9)

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Co1 | 0.0279 (3) | 0.0322 (3) | 0.0314 (3) | 0.0038 (2) | -0.0008 (2) | 0.0012 (2) |
| O1 | 0.0287 (15) | 0.0417 (17) | 0.0311 (15) | 0.0108 (12) | 0.0027 (12) | -0.0030 (13) |
| O2 | 0.0370 (16) | 0.0369 (16) | 0.0338 (16) | 0.0162 (14) | -0.0071 (13) | -0.0005 (13) |
| O3 | 0.0350 (16) | 0.0449 (18) | 0.0287 (16) | 0.0036 (14) | -0.0007 (13) | -0.0015 (13) |
| O4 | 0.0322 (16) | 0.0316 (15) | 0.0329 (15) | 0.0075 (12) | 0.0006 (13) | -0.0019 (12) |
| O5 | 0.0339 (16) | 0.0330 (15) | 0.0315 (15) | 0.0082 (13) | 0.0016 (13) | 0.0073 (12) |
| O6 | 0.0266 (14) | 0.0344 (16) | 0.0291 (14) | -0.0017 (13) | 0.0013 (12) | -0.0052 (12) |
| O7 | 0.0356 (16) | 0.0332 (15) | 0.0333 (15) | 0.0006 (13) | -0.0046 (13) | -0.0007 (12) |
| O8 | 0.0321 (15) | 0.0383 (16) | 0.0245 (15) | 0.0023 (13) | 0.0002 (12) | 0.0032 (12) |
| C1 | 0.025 (2) | 0.031 (2) | 0.030 (2) | 0.0022 (17) | -0.0002 (17) | 0.0009 (16) |
| C2 | 0.029 (2) | 0.030 (2) | 0.034 (2) | 0.0048 (18) | -0.0025 (18) | 0.0028 (17) |
| C3 | 0.028 (2) | 0.030 (2) | 0.030 (2) | 0.0009 (18) | 0.0028 (17) | -0.0004 (16) |
| C4 | 0.0257 (19) | 0.028 (2) | 0.0273 (19) | 0.0032 (16) | 0.0020 (17) | 0.0036 (16) |
| C5 | 0.027 (2) | 0.027 (2) | 0.033 (2) | -0.0014 (17) | 0.0005 (17) | 0.0039 (16) |
| C6 | 0.030 (2) | 0.036 (2) | 0.039 (2) | -0.0010 (19) | 0.0057 (19) | 0.0000 (19) |
| C7 | 0.026 (2) | 0.026 (2) | 0.037 (2) | -0.0021 (17) | -0.0026 (18) | 0.0006 (17) |
| C8 | 0.028 (2) | 0.034 (2) | 0.034 (2) | -0.0020 (18) | -0.0022 (18) | -0.0002 (18) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|-------------------------|-------------|-----------|-----------|
| Co1—O1 | 2.016 (3) | O7—H5 | 0.8889 |
| Co1—O7 | 2.044 (3) | O7—H6 | 0.8200 |
| Co1—O4 ⁱ | 2.076 (3) | O8—H3 | 0.8799 |
| Co1—O6 | 2.095 (3) | O8—H4 | 0.8200 |
| Co1—O8 | 2.112 (3) | C1—C2 | 1.391 (6) |
| Co1—O3 ⁱ | 2.324 (3) | C1—C6 | 1.399 (6) |
| O1—C7 | 1.258 (5) | C1—C7 | 1.510 (5) |
| O2—C7 | 1.249 (5) | C2—C3 | 1.384 (5) |
| O3—C8 | 1.264 (5) | C2—H7 | 0.9300 |
| O3—Co1 ⁱⁱ | 2.324 (3) | C3—C4 | 1.402 (5) |
| O4—C8 | 1.272 (5) | C3—C8 | 1.479 (6) |
| O4—Co1 ⁱⁱ | 2.076 (3) | C4—C5 | 1.385 (6) |
| O5—C5 | 1.374 (5) | C4—H8 | 0.9300 |
| O5—H9 | 0.8199 | C5—C6 | 1.367 (6) |
| O6—H1 | 0.8645 | C6—H10A | 0.9300 |
| O6—H2 | 0.8201 | | |
| O1—Co1—O7 | 94.93 (11) | Co1—O8—H4 | 109.4 |
| O1—Co1—O4 ⁱ | 108.64 (11) | H3—O8—H4 | 103.6 |
| O7—Co1—O4 ⁱ | 156.36 (11) | C2—C1—C6 | 119.7 (4) |
| O1—Co1—O6 | 89.68 (12) | C2—C1—C7 | 120.1 (4) |
| O7—Co1—O6 | 86.47 (11) | C6—C1—C7 | 120.2 (4) |
| O4 ⁱ —Co1—O6 | 95.36 (11) | C3—C2—C1 | 120.1 (4) |

| | | | |
|--------------------------------------|-------------|------------|-----------|
| O1—Co1—O8 | 93.16 (12) | C3—C2—H7 | 119.9 |
| O7—Co1—O8 | 86.82 (10) | C1—C2—H7 | 120.0 |
| O4 ⁱ —Co1—O8 | 89.89 (10) | C2—C3—C4 | 119.9 (4) |
| O6—Co1—O8 | 172.91 (10) | C2—C3—C8 | 122.0 (4) |
| O1—Co1—O3 ⁱ | 167.23 (10) | C4—C3—C8 | 118.1 (4) |
| O7—Co1—O3 ⁱ | 97.82 (10) | C5—C4—C3 | 119.2 (4) |
| O4 ⁱ —Co1—O3 ⁱ | 58.66 (10) | C5—C4—H8 | 120.4 |
| O6—Co1—O3 ⁱ | 90.33 (11) | C3—C4—H8 | 120.4 |
| O8—Co1—O3 ⁱ | 88.33 (11) | C6—C5—O5 | 121.9 (4) |
| C7—O1—Co1 | 138.0 (3) | C6—C5—C4 | 121.2 (4) |
| C8—O3—Co1 ⁱⁱ | 86.3 (2) | O5—C5—C4 | 116.9 (4) |
| C8—O4—Co1 ⁱⁱ | 97.6 (2) | C5—C6—C1 | 119.8 (4) |
| C5—O5—H9 | 109.6 | C5—C6—H10A | 120.3 |
| Co1—O6—H1 | 115.8 | C1—C6—H10A | 119.9 |
| Co1—O6—H2 | 109.5 | O2—C7—O1 | 124.8 (4) |
| H1—O6—H2 | 109.7 | O2—C7—C1 | 118.3 (4) |
| Co1—O7—H5 | 121.5 | O1—C7—C1 | 117.0 (4) |
| Co1—O7—H6 | 109.6 | O3—C8—O4 | 117.4 (4) |
| H5—O7—H6 | 110.5 | O3—C8—C3 | 123.1 (4) |
| Co1—O8—H3 | 113.5 | O4—C8—C3 | 119.5 (4) |

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

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| O5—H9 \cdots O3 ⁱⁱⁱ | 0.82 | 1.84 | 2.651 (4) | 172 |
| O6—H1 \cdots O5 ^{iv} | 0.86 | 1.86 | 2.720 (4) | 174 |
| O6—H2 \cdots O2 ^v | 0.82 | 1.85 | 2.655 (4) | 166 |
| O7—H5 \cdots O8 ^{vi} | 0.89 | 1.89 | 2.773 (4) | 173 |
| O7—H6 \cdots O6 ^{vii} | 0.82 | 2.17 | 2.913 (4) | 151 |
| O8—H3 \cdots O2 ^{viii} | 0.88 | 1.74 | 2.612 (4) | 170 |
| O8—H4 \cdots O4 ^{ix} | 0.82 | 1.86 | 2.634 (4) | 158 |

Symmetry codes: (iii) $-x+3/2, y, z-1/2$; (iv) $x+1/2, -y+1, -z+1/2$; (v) $-x+2, -y+1, -z+1$; (vi) $-x+2, y+1/2, -z+1/2$; (vii) $-x+2, y-1/2, -z+1/2$; (viii) $-x+2, -y, -z+1$; (ix) $-x+3/2, -y+1/2, z$.

Fig. 2

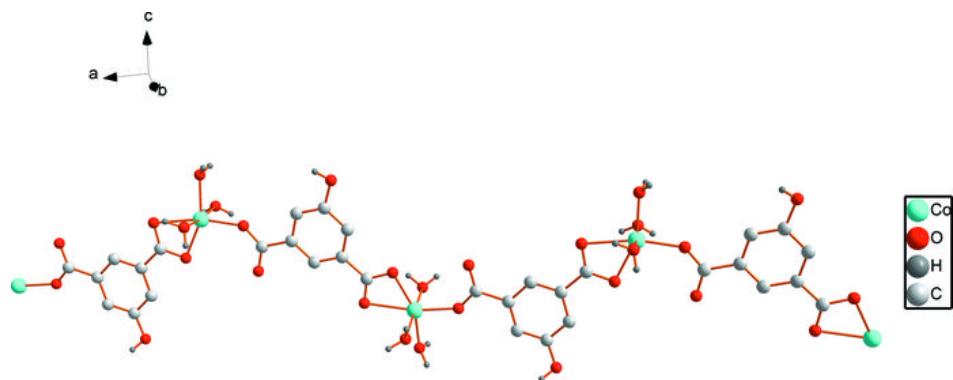


Fig. 3

