

Ming-Hua Zeng,<sup>a</sup> Yan-Ling Zhou<sup>a</sup>  
and Seik Weng Ng<sup>b\*</sup>

<sup>a</sup>School of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

#### Key indicators

Single-crystal X-ray study

$T = 295$  K

Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å

$R$  factor = 0.028

$wR$  factor = 0.068

Data-to-parameter ratio = 12.9

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## catena-Poly[[diaqua[(*Z*)-3-(1*H*-benzimidazol-2-yl)prop-2-enoato- $\kappa^2\text{N},\text{O}$ ]cobalt(II)]- $\mu$ -(*Z*)-3-(1*H*-benzimidazol-2-yl)prop-2-enoato- $\kappa^2\text{O}:\text{O}'$ ]

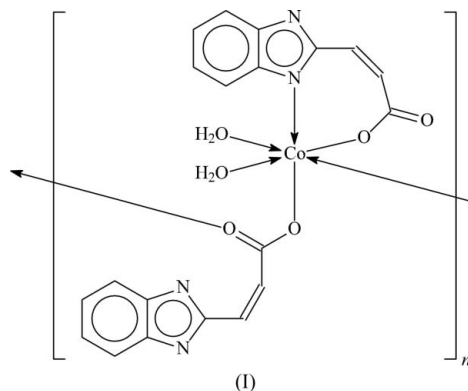
In the title compound,  $[\text{Co}(\text{C}_{10}\text{H}_7\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2]_n$ , the  $\text{Co}^{\text{II}}$  atom is hexacoordinated in a distorted octahedral geometry by five O atoms [ $\text{Co}-\text{O} = 2.074(2)$ – $2.200(2)$  Å] and one N atom [ $\text{Co}-\text{N} = 2.114(2)$  Å]. One 3-(1*H*-benzimidazol-2-yl)prop-2-enoate anion chelates to  $\text{Co}^{\text{II}}$  through N and O, whereas the other functions as a carboxylate bridge, linking the *cis*-water-coordinated metal atoms into a zigzag chain that runs along the *a* axis of the orthorhombic unit cell. The chains are consolidated into a three-dimensional network by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

Received 26 July 2006

Accepted 2 August 2006

#### Comment

(*Z*)-3-(1*H*-Benzimidazol-2-yl)prop-2-enoic acid is a carboxylic acid having an *N*-heterocyclic substituent that possesses Lewis basic and hydrogen-donor sites. A literature search (SciFinder, 2006) has shown that the acid has not been used in the synthesis of metal carboxylates. We present here the crystal structure of the title compound, (I), which is a cobalt derivative of the aforementioned acid.



In (I), the  $\text{Co}^{\text{II}}$  atom is hexacoordinated (Fig. 1) in a distorted octahedral geometry by five O atoms and one N atom (Table 1). The water molecules are *cis* to each other in an octahedral environment. One 3-(1*H*-benzimidazol-2-yl)prop-2-enoate anion behaves as a chelate, whereas the other functions as a carboxylate bridge (Fig. 1). The bridging mode leads to a polymeric zigzag chain that runs along the *a* axis of the orthorhombic unit cell. Adjacent polymeric chains are linked by intermolecular hydrogen bonds (Table 2) into a three-dimensional network structure.

#### Experimental

(*Z*)-3-(1*H*-Benzimidazol-2-yl)prop-2-enoic acid was synthesized using a modification (Ying & Dai, 1993) of an older literature

procedure (Phillips, 1928). To a solution of cobalt(II) nitrate hexahydrate (0.29 g, 1 mmol) in water (5 ml) was added an aqueous solution (5 ml) of the acid (0.38 g, 2 mmol). The solution was warmed to 333 K to ensure complete dissolution of the reagents. Red block-shaped crystals were separated from the solution after two weeks (yield 70%).

Crystal data

[Co(C<sub>10</sub>H<sub>7</sub>N<sub>2</sub>O<sub>2</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]  
*M<sub>r</sub>* = 469.31  
 Orthorhombic, *Pca*2<sub>1</sub>  
*a* = 8.9808 (5) Å  
*b* = 12.1341 (7) Å  
*c* = 17.873 (1) Å  
*V* = 1947.7 (2) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.601 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 μ = 0.93 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Block, red  
 0.30 × 0.20 × 0.17 mm

Data collection

Bruker SMART area-detector diffractometer  
 φ and ω scans  
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.800, *T<sub>max</sub>* = 0.854

14505 measured reflections  
 3814 independent reflections  
 3325 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.032  
 θ<sub>max</sub> = 26.0°

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.028  
*wR* (*F*<sup>2</sup>) = 0.068  
*S* = 1.01  
 3814 reflections  
 296 parameters  
 H atoms treated by a mixture of independent and constrained refinement

*w* = 1/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0367*P*)<sup>2</sup> + 0.2415*P*]  
 where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3  
 (Δσ)<sub>max</sub> = 0.001  
 Δρ<sub>max</sub> = 0.21 e Å<sup>-3</sup>  
 Δρ<sub>min</sub> = -0.24 e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), with 1835 Friedel pairs  
 Flack parameter: -0.02 (1)

Table 1

Selected geometric parameters (Å, °).

Co1—O1	2.074 (2)	Co1—O1w	2.088 (2)
Co1—O2 <sup>i</sup>	2.099 (2)	Co1—O2w	2.094 (2)
Co1—O3	2.200 (2)	Co1—N1	2.114 (2)
O1—Co1—O2 <sup>i</sup>	81.0 (1)	O2 <sup>i</sup> —Co1—N1	93.8 (1)
O1—Co1—O3	94.0 (1)	O3—Co1—O1w	87.9 (1)
O1—Co1—O1w	178.0 (1)	O3—Co1—O2w	85.9 (1)
O1—Co1—O2w	90.5 (1)	O3—Co1—N1	92.7 (1)
O1—Co1—N1	88.3 (1)	O1w—Co1—O2w	89.1 (1)
O2 <sup>i</sup> —Co1—O3	171.7 (1)	O1w—Co1—N1	92.2 (1)
O2 <sup>i</sup> —Co1—O1w	97.0 (1)	O2w—Co1—N1	178.1 (1)
O2 <sup>i</sup> —Co1—O2w	87.6 (1)		

Symmetry code: (i) *x* + ½, -*y* + 2, *z*.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1w—H1w1...N4 <sup>ii</sup>	0.84 (3)	2.04 (3)	2.868 (3)	167 (3)
O1w—H1w2...O1 <sup>i</sup>	0.85 (3)	2.37 (3)	2.918 (2)	123 (3)
O2w—H2w1...O4	0.84 (3)	1.77 (3)	2.613 (3)	176 (4)
N2—H2 <i>n</i> ...O4 <sup>iii</sup>	0.85	2.04	2.757 (3)	141
N3—H3 <i>n</i> ...O3	0.85	1.91	2.653 (3)	145

Symmetry codes: (i) *x* + ½, -*y* + 2, *z*; (ii) *x* + ½, -*y* + 1, *z*; (iii) -*x* + ¾, *y*, *z* + ½.

The C- and N-bound H atoms were placed in calculated positions (C—H = 0.93 Å and N—H = 0.85 Å) and included in the refinement in

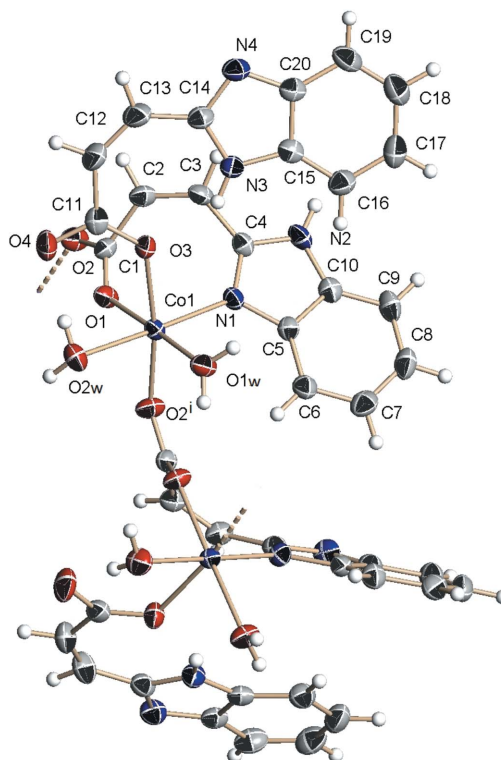


Figure 1

The structure of a portion of the polymeric chain in (I), showing displacement ellipsoids drawn at the 50% probability level and the atomic labelling [symmetry code: (i) ½ + *x*, 2 - *y*, *z*].

the riding-model approximation, with *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C,N). The water H atoms were located in a difference Fourier map and isotropically refined with distance restraints of O—H = 0.85 (1) Å and H...H = 1.39 (1) Å. The O2w water molecule forms only one hydrogen bond; the possibility that this unit is an OH group was discounted as two H atoms were clearly observed in a difference Fourier map and refined.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the Natural Science Foundation of Guangxi Province (grant No. 0447019) and the University of Malaya for supporting of this study.

References

Bruker (1999). *SAINTE* (Version 6.45A) and *SMART* (Version 6.45A). Bruker AXS Inc, Madison, Wisconsin, USA.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
 Phillips, M. A. (1928). *J. Chem. Soc.* pp. 172–177.  
 SciFinder (2006). American Chemical Society, USA.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Ying, H.-Q. & Dai, X.-F. (1993). *Yaoxue Xuebao*, **28**, 553–556. (In Chinese.)