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Key indicators

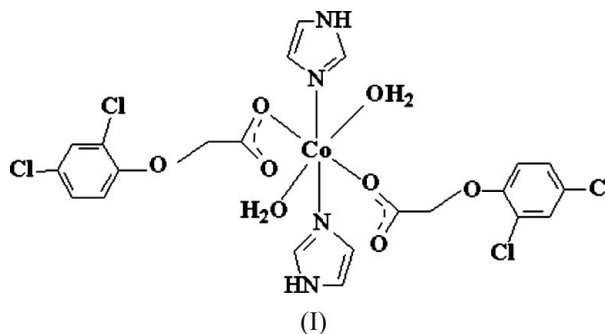
Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.031
 wR factor = 0.080
Data-to-parameter ratio = 16.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Diaquabis(2,4-dichlorophenoxyacetato- κO)-
bis(1*H*-imidazole- κN^3)cobalt(II)

The Co^{II} atom in the mononuclear title complex, $[\text{Co}(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_3)_2(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_2]$, lies on an inversion center. The Co^{II} atom has an octahedral coordination, involving two carboxylate O atoms of two monodentate 2,4-dichlorophenoxyacetate ligands, two N atoms of imidazole ligands and two water molecules. Intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds give rise to chains, which are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a sheet structure. The molecules are further linked by $\pi-\pi$ stacking interactions, generating a two-dimensional supramolecular network.

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Comment

2,4-Dichlorophenoxyacetic acid is an extremely important biologically active compound, that has been commonly used in herbicides and plant-growth agents (Lv, 1998). The monophenoxyacetate group has versatile bonding modes to metal ions and easily forms simple complexes (Liang *et al.*, 2002). The reaction system of cobalt diacetate trihydrate, imidazole and 2,4-dichlorophenoxyacetic acid has therefore been explored; this leads to a new mononuclear complex, (I), the crystal structure of which is reported here.



As shown in Fig. 1, the Co^{II} atom exists in an octahedral coordination environment, defined by two carboxylate O atoms of the monodentate 2,4-dichlorophenoxyacetate ligands, two N atoms of two imidazole ligands and two water molecules (see Table 1). The Co^{II} atom lies on an inversion center. The oxyacetate group is clearly twisted out of the plane of the benzene ring in (I), the $\text{C}3-\text{O}3-\text{C}2-\text{C}1$ torsion angle being $-66.6(2)^\circ$. The characteristic $\text{C}-\text{O}$ (carboxylate) bond lengths (Table 1) suggest electron delocalization of the carboxylate groups of the anionic ligands.

In each of the mononuclear units, an intramolecular hydrogen bond is formed between the uncoordinated carboxylate O2 atom and the coordinated water molecule (O1W) (see Table 2). An intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen

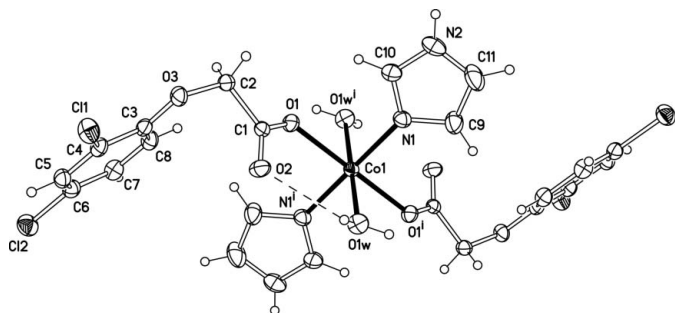


Figure 1
Molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $-x + 1, -y + 1, -z$.]

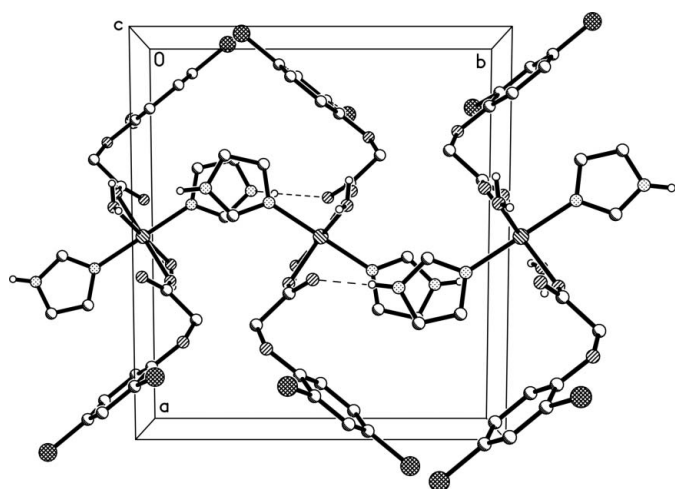


Figure 2
An N—H...O hydrogen-bonded (dashed lines) chain in(I). H atoms not involved in hydrogen bonding have been omitted.

bond is also formed between O1W and a symmetry-equivalent O2 atom, leading to a chain parallel to the *c* axis. An intermolecular N—H...O hydrogen bond is formed between the uncoordinated carboxylate atom O2 and the imidazole atom N5, leading to a hydrogen-bonded chain parallel to the *b* axis (for details, see Table 2 and Fig. 2). The chains crosslink each other and are further linked through π – π stacking interactions between imidazole molecules at 3.804 (2) Å, giving rise to a two-dimensional supramolecular network (for details, see Table 2 and Fig. 3).

Experimental

2,4-Dichlorophenoxyacetic acid was synthesized from hydrochloric acid, hydrogen peroxide and sodium hypochlorite (Wu *et al.*, 1996). Cobalt diacetate trihydrate (4.76 g, 20 mmol), imidazole (1.36 g, 20 mmol) and 2,4-dichlorophenoxyacetic acid (4.42 g, 20 mmol) were dissolved in a 1:5 ethanol–water solution and then the pH was adjusted to 7 with 0.2 M sodium hydroxide. The resulting solution was stirred for 30 min at room temperature and then filtered. Colorless single crystals were isolated from the solution at room temperature over several days. Analysis calculated for $C_{22}H_{22}Cl_4CoN_4O_8$: C 39.37, H 3.30, N 8.35%; found: C 39.42, H 3.34, N 8.34%.

Crystal data

$[Co(C_8H_5Cl_2O_3)_2(C_3H_4N_2)_2(H_2O)_2]$
 $M_r = 671.17$
Monoclinic, $P2_1/c$
 $a = 14.137$ (3) Å
 $b = 12.720$ (3) Å
 $c = 7.5265$ (15) Å
 $\beta = 98.93$ (3)°
 $V = 1337.0$ (5) Å³

$Z = 2$
 $D_x = 1.667$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 1.10$ mm⁻¹
 $T = 295$ (2) K
Block, colorless
 $0.35 \times 0.24 \times 0.18$ mm

Data collection

Rigaku R-Axis RAPID
diffractometer
 ω scans
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{min} = 0.700$, $T_{max} = 0.827$

12406 measured reflections
3064 independent reflections
2658 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.031$
 $\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.080$
 $S = 1.06$
3064 reflections
184 parameters
H atoms treated by a mixture of
independent and constrained
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 0.3243P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.37$ e Å⁻³
 $\Delta\rho_{min} = -0.25$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|-------------------------|-------------|---------------------------|-------------|
| Co1—N1 | 2.0895 (14) | Cl2—C6 | 1.7426 (18) |
| Co1—O1 | 2.1524 (12) | O1—C1 | 1.2546 (19) |
| Co1—O1W | 2.1631 (14) | O2—C1 | 1.246 (2) |
| Cl1—C4 | 1.7368 (18) | | |
| N1—Co1—N1 ⁱ | 180 | O1 ⁱ —Co1—O1 | 180 |
| N1—Co1—O1 ⁱ | 92.09 (5) | O1—Co1—O1W | 99.38 (5) |
| N1—Co1—O1 | 87.91 (5) | O1—Co1—O1W ⁱ | 80.62 (5) |
| N1—Co1—O1W ⁱ | 88.12 (6) | O1W ⁱ —Co1—O1W | 180 |
| N1—Co1—O1W | 91.88 (6) | | |

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

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> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| N2—H2N...O2 ⁱⁱ | 0.86 | 1.93 | 2.790 (2) | 178 |
| O1W—H1W1...O2 ⁱⁱⁱ | 0.843 (9) | 2.019 (14) | 2.8072 (19) | 155 (2) |
| O1W—H1W1...O2 | 0.843 (9) | 2.503 (19) | 3.002 (2) | 118.8 (17) |

Symmetry codes: (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ (iii) $-x + 1, -y + 1, -z + 1$.

C-bound H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 Å (aliphatic) and $U_{iso}(H) = 1.2U_{eq}(C)$, and were refined in the riding-model approximation. The H atoms of the water molecule and imidazole were located in a difference map and refined with O—H, H...H and N—H distance restraints of 0.85 (1), 1.39 (1) and 0.90 (1) Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}(O,N)$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); 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*.

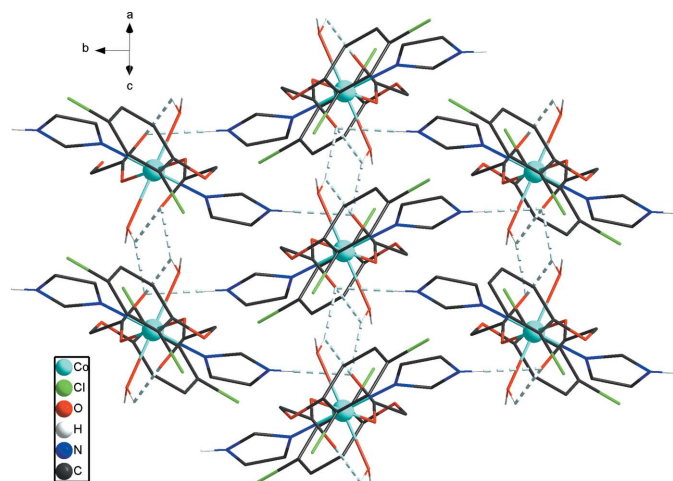


Figure 3
Packing diagram of (I). Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

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