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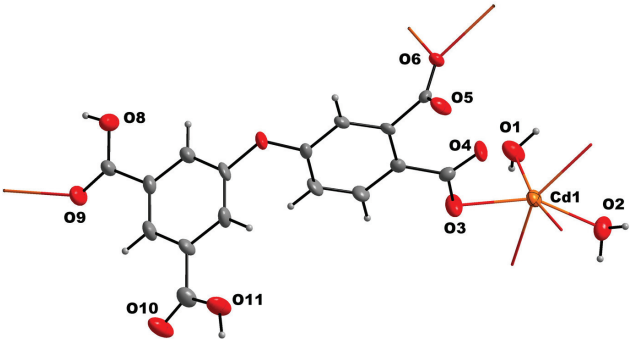
# Crystal structure of *poly*[*diaqua*-(μ$_4$-4-(3,5-dicarboxy-κ$^1$*O*-phenoxy)phthalato-κ$^3$*O*:*O*′:*O*′) cadmium(II)], $C_{16}H_{12}CdO_{11}$




https://doi.org/10.1515/ncrs-2019-0407
Received June 13, 2019; accepted August 26, 2019; available online September 14, 2019

## Abstract

$C_{16}H_{12}CdO_{11}$, monoclinic, $P2_1/c$ (no. 14), $a = 14.6977(6)$ Å, $b = 5.9706(2)$ Å, $c = 20.7220(10)$ Å, $\beta = 109.802(5)°$, $V = 1710.91(13)$ Å$^3$, $Z = 4$, $R_{gt}(F) = 0.0456$, $wR_{ref}(F^2) = 0.1583$, $T = 296(2)$ K.

**CCDC no.:** 1949282

A part of the title structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

## Source of material

A mixture of 5-(3′,4′-dicarboxylphenoxy)-isophthalic acid (35 mg, 0.1 mmol), and $Cd(NO_3)_2{\cdot}6H_2O$ (29.1 mg, 0.1 mmol), were added to water (10 mL) in a 25 mL Teflon-lined autoclave. The mixture was heated at 423 K for 3 days and then slowly cooled down to room temperature. Red block crystals of the title compound were obtained.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Red block |
| Size: | 0.42 × 0.32 × 0.26 mm |
| Wavelength: | Mo *Kα* radiation (0.71073 Å) |
| $\mu$: | 1.34 mm$^{-1}$ |
| Diffractometer, scan mode: | SuperNova, $\omega$ |
| $\theta_{max}$, completeness: | 25.5°, >99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 18198, 3178, 0.052 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\,\sigma(I_{obs})$, 2916 |
| $N(param)_{refined}$: | 257 |
| Programs: | Bruker [1], SHELX [2, 3] |

## Experimental details

The hydrogen atoms were placed in calculated positions riding on attached atoms with isotropic thermal parameters.

## Comment

In recent years, research on coordination complexes has made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and functional applications, such as catalysis, luminescence, gas storage, magnetism, molecular separation and sensors [4–7]. It is well known that organic ligands play crucial roles in the design and construction of desirable frameworks [8–10]. And for this purpose, numerous multifunctional carboxylate ligands have been designed, synthesized and investigated deeply, owing to their inherent outstanding coordination capabilities and changeable coordination modes [11, 12]. The semi-rigid multicarboxylate ligand 3-(3,5-dicarboxyphenoxy)phthalic acid has eight possible coordination sites which can supply varied patterns (monodentate, bridging, chelating) to construct coordination polymers. The asymmetric unit of the title structure contains Cd(II) ion and 5-(3′,4′-dicarboxylphenoxy)-isophthalate dianion as ligand to construct a new 2D coordination polymer. The cadmium atom Cd1 is six-coordinated by four oxygen atoms from 5-(3′,4′-dicarboxylphenoxy)-isophthalate ligands and two oxygen atoms from coordinated water molecules. The Cd—O bond lengths range from 2.290(4) to 2.416(4) Å and are in the expected ranges [13]. This compound exhibits a 3D structure through hydrogen bonds.

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.07442(3) | 0.05569(6) | 0.590967(19) | 0.0217(2) |
| O1 | 0.0404(3) | 0.2665(7) | 0.6729(2) | 0.0381(10) |
| H1A | 0.0594 | 0.1977 | 0.7125 | 0.057* |
| H1B | −0.0220 | 0.2779 | 0.6633 | 0.057* |
| O2 | −0.0064(3) | −0.2622(7) | 0.6020(2) | 0.0359(10) |
| H2A | 0.0338 | −0.3720 | 0.6178 | 0.054* |
| H2B | −0.0426 | −0.3094 | 0.5619 | 0.054* |
| O3 | 0.2155(3) | 0.2564(7) | 0.6226(2) | 0.0363(10) |
| O4 | 0.1131(3) | 0.4061(6) | 0.5318(2) | 0.0353(11) |
| O5 | 0.1391(3) | 0.7247(7) | 0.41855(19) | 0.0296(9) |
| O6 | 0.0794(2) | 0.8885(6) | 0.49060(19) | 0.0189(8) |
| O7 | 0.4668(3) | 1.0787(6) | 0.5822(2) | 0.0284(10) |
| O8 | 0.6795(3) | 1.5397(6) | 0.7724(3) | 0.0355(11) |
| H8 | 0.7067 | 1.6253 | 0.8040 | 0.053* |
| O9 | 0.8182(3) | 1.3466(7) | 0.8137(2) | 0.0336(10) |
| O10 | 0.8578(3) | 0.6499(9) | 0.6915(2) | 0.0460(12) |
| O11 | 0.7450(3) | 0.5875(8) | 0.5895(2) | 0.0415(12) |
| H11 | 0.7755 | 0.4710 | 0.5917 | 0.062* |
| C1 | 0.1933(4) | 0.4061(8) | 0.5768(3) | 0.0208(12) |
| C2 | 0.2660(4) | 0.5838(8) | 0.5789(3) | 0.0178(11) |
| C3 | 0.3582(4) | 0.5740(9) | 0.6273(3) | 0.0252(13) |
| H3 | 0.3738 | 0.4557 | 0.6583 | 0.030* |
| C4 | 0.4273(4) | 0.7333(9) | 0.6309(3) | 0.0272(12) |
| H4 | 0.4885 | 0.7242 | 0.6641 | 0.033* |
| C5 | 0.4039(4) | 0.9080(8) | 0.5841(3) | 0.0203(11) |
| C6 | 0.3126(4) | 0.9237(8) | 0.5359(3) | 0.0193(11) |
| H6 | 0.2975 | 1.0433 | 0.5053 | 0.023* |
| C7 | 0.2432(3) | 0.7636(8) | 0.5325(2) | 0.0160(10) |
| C8 | 0.1462(3) | 0.7896(8) | 0.4770(3) | 0.0169(10) |
| C9 | 0.5630(4) | 1.0607(8) | 0.6236(3) | 0.0256(13) |
| C10 | 0.6215(4) | 0.8939(10) | 0.6122(3) | 0.0273(13) |
| H10 | 0.5972 | 0.7921 | 0.5765 | 0.033* |
| C11 | 0.7174(4) | 0.8821(10) | 0.6553(3) | 0.0216(11) |
| C12 | 0.7536(4) | 1.0367(9) | 0.7082(3) | 0.0241(12) |
| H12 | 0.8170 | 1.0248 | 0.7382 | 0.029* |
| C13 | 0.6954(4) | 1.2063(9) | 0.7158(3) | 0.0239(12) |
| C14 | 0.5989(4) | 1.2160(9) | 0.6747(3) | 0.0250(12) |
| H14 | 0.5588 | 1.3269 | 0.6818 | 0.030* |
| C15 | 0.7375(4) | 1.3724(9) | 0.7725(3) | 0.0241(12) |
| C16 | 0.7815(4) | 0.6991(10) | 0.6472(3) | 0.0295(13) |

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