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# Tetraaquabis[2-(2,4-dichlorophenoxy)-acetato]nickel(II)

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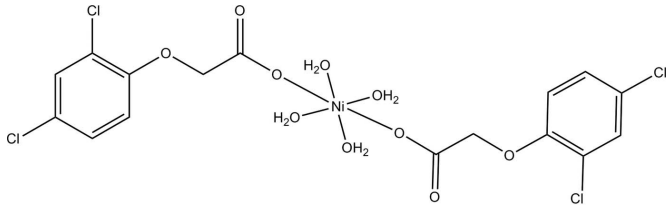
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.010 Å; $R$ factor = 0.071; $wR$ factor = 0.214; data-to-parameter ratio = 12.8.

In the title complex, $[Ni(C_8H_5Cl_2O_3)_2(H_2O)_4]$, the $Ni^{II}$ atom (site symmetry $\overline{1}$) adopts a slightly distorted $NiO_6$ octahedral coordination. An intramolecular O—H···O hydrogen bond helps to establish the conformation. In the crystal, further O—H···O hydrogen bonds link the molecules.

## Related literature

For background, see: Cheng *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$[Ni(C_8H_5Cl_2O_3)_2(H_2O)_4]$
$M_r$ = 570.81
Monoclinic, $P2_1/c$
$a$ = 16.860 (3) Å
$b$ = 8.1370 (16) Å
$c$ = 8.3010 (17) Å
$\beta$ = 95.87 (3)°
$V$ = 1132.8 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.38 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.683, $T_{max}$ = 0.875
2134 measured reflections
1976 independent reflections
1596 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017
200 standard reflections
every 3 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.214
$S$ = 1.14
1976 reflections
154 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.86 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.97 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ni1—O3 | 2.085 (5) | Ni1—O1 | 2.130 (4) |
| Ni1—O4 | 2.126 (4) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···O2$^{i}$ | 0.84 (5) | 2.05 (7) | 2.723 (7) | 136 (8) |
| O1—H1$B$···O2 | 0.84 (3) | 1.82 (5) | 2.619 (7) | 157 (7) |
| O3—H3$A$···O1$^{i}$ | 0.85 (6) | 2.44 (7) | 3.217 (7) | 153 (7) |
| O3—H3$B$···O6$^{ii}$ | 0.846 (16) | 2.34 (6) | 2.980 (7) | 133 (8) |

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB5064).

## References

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# supporting information

*Acta Cryst.* (2009). E**65**, m1148 [doi:10.1107/S1600536809033662]

## Tetraaquabis[2-(2,4-dichlorophenoxy)acetato]nickel(II)

**Wu Chen, Ji-Wen Yuan, Lei Lei and Qing-Fu Zeng**

### S1. Comment

There has been much research interest in acid metal complexes due to their molecular architectures and biological activities (e.g. Cheng *et al.*, 2006). In this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The $Ni^{II}$ atom is six-coordinated by two O atoms from the 2-(2,4-dichlorophenoxy)acetate and four O atoms from the water molecules, forming a slightly distorted octahedral coordination.

### S2. Experimental

A mixture of 2-(2,4-dichlorophenoxy)acetic acid (440 mg, 2 mmol) and NiCl2.6H2O (1 mmol, 236 mg) in methanol (10 ml) was stirred for 3 h. After keeping the filtrate in air for 7 d, green blocks of (I) were formed.

### S3. Refinement

The water H atoms were located in a difference map and their positions were refined with the restraint O—H = 0.83 (1)Å. The other H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

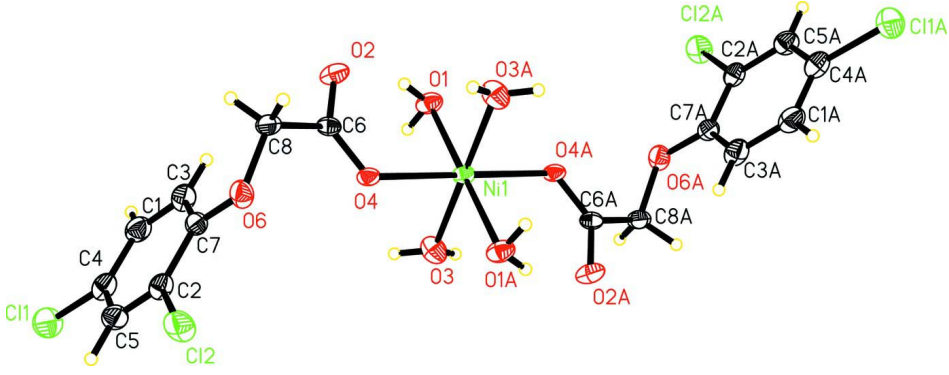


**Figure 1**

The molecular structure of (I) showing 30% probability displacement ellipsoids. Atoms with the suffix A are generated by the symmetry operation (1–x, –y, 1–z).

### Tetraaquabis[2-(2,4-dichlorophenoxy)acetato]nickel(II)

*Crystal data*

$[Ni(C_8H_5Cl_2O_3)_2(H_2O)_4]$
$M_r$ = 570.81
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 16.860 (3) Å
$b$ = 8.1370 (16) Å
$c$ = 8.3010 (17) Å
$\beta$ = 95.87 (3)°
$V$ = 1132.8 (4) Å$^3$
$Z$ = 2

$F(000) = 580$
$D_x = 1.673$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–12°$
$\mu = 1.38$ mm$^{-1}$
$T = 293$ K
Block, green
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.683$, $T_{max} = 0.875$
2134 measured reflections
1976 independent reflections
1596 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.2°$, $\theta_{min} = 1.2°$
$h = -20 \rightarrow 20$
$k = -9 \rightarrow 0$
$l = 0 \rightarrow 9$
200 standard reflections every 3 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.214$
$S = 1.14$
1976 reflections
154 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1181P)^2 + 3.965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.86$ e Å$^{-3}$
$\Delta\rho_{min} = -1.97$ e Å$^{-3}$

*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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.1103 (4) | 0.1141 (9) | 0.3299 (9) | 0.0487 (17) |
| H1 | 0.0872 | 0.0160 | 0.3585 | 0.058* |
| C2 | 0.1780 (4) | 0.4056 (8) | 0.2486 (8) | 0.0363 (14) |
| C3 | 0.1822 (4) | 0.1110 (8) | 0.2642 (9) | 0.0454 (16) |
| H3 | 0.2076 | 0.0113 | 0.2504 | 0.054* |
| C4 | 0.0724 (4) | 0.2598 (9) | 0.3534 (9) | 0.0458 (16) |
| C5 | 0.1072 (4) | 0.4079 (8) | 0.3131 (8) | 0.0431 (15) |
| H5 | 0.0821 | 0.5072 | 0.3303 | 0.052* |
| C6 | 0.3693 (4) | 0.0240 (7) | 0.2247 (7) | 0.0296 (12) |
| C7 | 0.2173 (4) | 0.2580 (7) | 0.2183 (8) | 0.0345 (13) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.3201 (4) | 0.1188 (8) | 0.0942 (7) | 0.0388 (15) |
| H8A | 0.3533 | 0.1447 | 0.0088 | 0.047* |
| H8B | 0.2770 | 0.0489 | 0.0479 | 0.047* |
| Cl1 | −0.01949 (12) | 0.2621 (3) | 0.4316 (3) | 0.0626 (6) |
| Cl2 | 0.22352 (11) | 0.5880 (2) | 0.1988 (3) | 0.0557 (6) |
| H1A | 0.418 (3) | −0.233 (12) | 0.523 (6) | 0.067* |
| H3A | 0.452 (4) | −0.018 (10) | 0.785 (6) | 0.067* |
| H1B | 0.436 (4) | −0.226 (11) | 0.366 (3) | 0.067* |
| H3B | 0.3858 (7) | 0.030 (11) | 0.687 (9) | 0.067* |
| Ni1 | 0.5000 | 0.0000 | 0.5000 | 0.0266 (4) |
| O1 | 0.4550 (3) | −0.2430 (5) | 0.4624 (6) | 0.0406 (11) |
| O2 | 0.3738 (3) | −0.1289 (5) | 0.2003 (5) | 0.0433 (11) |
| O3 | 0.4362 (3) | 0.0347 (7) | 0.6996 (6) | 0.0503 (12) |
| O4 | 0.4045 (2) | 0.0994 (5) | 0.3429 (5) | 0.0319 (9) |
| O6 | 0.2866 (3) | 0.2687 (6) | 0.1489 (6) | 0.0420 (11) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.053 (4) | 0.039 (4) | 0.052 (4) | −0.005 (3) | −0.005 (3) | −0.005 (3) |
| C2 | 0.038 (3) | 0.029 (3) | 0.041 (3) | −0.008 (3) | −0.002 (3) | 0.005 (3) |
| C3 | 0.048 (4) | 0.027 (3) | 0.059 (4) | −0.002 (3) | −0.009 (3) | 0.004 (3) |
| C4 | 0.049 (4) | 0.046 (4) | 0.040 (4) | −0.006 (3) | −0.006 (3) | 0.002 (3) |
| C5 | 0.049 (4) | 0.032 (3) | 0.047 (4) | 0.000 (3) | 0.000 (3) | 0.000 (3) |
| C6 | 0.039 (3) | 0.018 (3) | 0.032 (3) | 0.001 (2) | 0.006 (2) | −0.002 (2) |
| C7 | 0.037 (3) | 0.029 (3) | 0.036 (3) | 0.004 (2) | −0.004 (2) | 0.000 (2) |
| C8 | 0.046 (4) | 0.035 (3) | 0.034 (3) | 0.006 (3) | −0.001 (3) | −0.009 (3) |
| Cl1 | 0.0543 (11) | 0.0675 (13) | 0.0680 (13) | −0.0061 (9) | 0.0147 (9) | −0.0037 (10) |
| Cl2 | 0.0552 (11) | 0.0276 (8) | 0.0841 (14) | 0.0013 (7) | 0.0062 (9) | 0.0059 (8) |
| Ni1 | 0.0369 (6) | 0.0154 (5) | 0.0270 (6) | 0.0015 (4) | 0.0017 (4) | 0.0023 (4) |
| O1 | 0.058 (3) | 0.028 (2) | 0.035 (2) | 0.000 (2) | −0.001 (2) | −0.0015 (19) |
| O2 | 0.066 (3) | 0.031 (2) | 0.032 (2) | −0.001 (2) | −0.003 (2) | −0.0056 (18) |
| O3 | 0.048 (3) | 0.054 (3) | 0.050 (3) | 0.009 (2) | 0.013 (2) | 0.007 (2) |
| O4 | 0.043 (2) | 0.0205 (19) | 0.030 (2) | 0.0092 (17) | −0.0054 (17) | −0.0048 (17) |
| O6 | 0.037 (2) | 0.032 (2) | 0.056 (3) | 0.0010 (18) | −0.002 (2) | 0.004 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C4 | 1.369 (10) | C7—O6 | 1.358 (8) |
| C1—C3 | 1.381 (11) | C8—O6 | 1.437 (7) |
| C1—H1 | 0.9300 | C8—H8A | 0.9700 |
| C2—C5 | 1.358 (10) | C8—H8B | 0.9700 |
| C2—C7 | 1.407 (9) | Ni1—O3 | 2.085 (5) |
| C2—Cl2 | 1.740 (6) | Ni1—O3$^{i}$ | 2.085 (5) |
| C3—C7 | 1.403 (9) | Ni1—O4 | 2.126 (4) |
| C3—H3 | 0.9300 | Ni1—O4$^{i}$ | 2.126 (4) |
| C4—C5 | 1.396 (10) | Ni1—O1$^{i}$ | 2.130 (4) |
| C4—Cl1 | 1.741 (8) | Ni1—O1 | 2.130 (4) |

| | | | |
|---|---|---|---|
| C5—H5 | 0.9300 | O1—H1A | 0.841 (10) |
| C6—O4 | 1.253 (7) | O1—H1B | 0.840 (10) |
| C6—O2 | 1.265 (7) | O3—H3A | 0.844 (10) |
| C6—C8 | 1.508 (8) | O3—H3B | 0.847 (10) |
| | | | |
| C4—C1—C3 | 120.9 (7) | C6—C8—H8B | 108.7 |
| C4—C1—H1 | 119.6 | H8A—C8—H8B | 107.6 |
| C3—C1—H1 | 119.6 | O3—Ni1—O3$^{i}$ | 180.0 |
| C5—C2—C7 | 122.1 (6) | O3—Ni1—O4 | 90.93 (19) |
| C5—C2—Cl2 | 120.6 (5) | O3$^{i}$—Ni1—O4 | 89.07 (18) |
| C7—C2—Cl2 | 117.3 (5) | O3—Ni1—O4$^{i}$ | 89.07 (18) |
| C1—C3—C7 | 120.2 (6) | O3$^{i}$—Ni1—O4$^{i}$ | 90.93 (18) |
| C1—C3—H3 | 119.9 | O4—Ni1—O4$^{i}$ | 180.0 |
| C7—C3—H3 | 119.9 | O3—Ni1—O1$^{i}$ | 87.9 (2) |
| C1—C4—C5 | 120.0 (7) | O3$^{i}$—Ni1—O1$^{i}$ | 92.1 (2) |
| C1—C4—Cl1 | 120.5 (6) | O4—Ni1—O1$^{i}$ | 88.46 (16) |
| C5—C4—Cl1 | 119.5 (6) | O4$^{i}$—Ni1—O1$^{i}$ | 91.54 (16) |
| C2—C5—C4 | 119.4 (6) | O3—Ni1—O1 | 92.1 (2) |
| C2—C5—H5 | 120.3 | O3$^{i}$—Ni1—O1 | 87.9 (2) |
| C4—C5—H5 | 120.3 | O4—Ni1—O1 | 91.54 (16) |
| O4—C6—O2 | 125.2 (5) | O4$^{i}$—Ni1—O1 | 88.46 (16) |
| O4—C6—C8 | 119.6 (5) | O1$^{i}$—Ni1—O1 | 180.0 |
| O2—C6—C8 | 115.2 (5) | Ni1—O1—H1A | 96 (7) |
| O6—C7—C3 | 125.1 (6) | Ni1—O1—H1B | 94 (6) |
| O6—C7—C2 | 117.5 (5) | H1A—O1—H1B | 108.9 (18) |
| C3—C7—C2 | 117.4 (6) | Ni1—O3—H3A | 117 (6) |
| O6—C8—C6 | 114.4 (5) | Ni1—O3—H3B | 119 (6) |
| O6—C8—H8A | 108.7 | H3A—O3—H3B | 108.4 (18) |
| C6—C8—H8A | 108.7 | C6—O4—Ni1 | 124.2 (4) |
| O6—C8—H8B | 108.7 | C7—O6—C8 | 117.5 (5) |
| | | | |
| C4—C1—C3—C7 | −0.9 (11) | O4—C6—C8—O6 | −28.4 (8) |
| C3—C1—C4—C5 | −1.0 (11) | O2—C6—C8—O6 | 154.2 (6) |
| C3—C1—C4—Cl1 | 178.4 (5) | O2—C6—O4—Ni1 | 14.9 (9) |
| C7—C2—C5—C4 | 1.0 (10) | C8—C6—O4—Ni1 | −162.2 (4) |
| Cl2—C2—C5—C4 | −179.3 (5) | O3—Ni1—O4—C6 | −122.0 (5) |
| C1—C4—C5—C2 | 0.9 (10) | O3$^{i}$—Ni1—O4—C6 | 58.0 (5) |
| Cl1—C4—C5—C2 | −178.5 (5) | O4$^{i}$—Ni1—O4—C6 | 76 (100) |
| C1—C3—C7—O6 | −178.2 (6) | O1$^{i}$—Ni1—O4—C6 | 150.1 (5) |
| C1—C3—C7—C2 | 2.7 (10) | O1—Ni1—O4—C6 | −29.9 (5) |
| C5—C2—C7—O6 | 178.0 (6) | C3—C7—O6—C8 | 10.6 (9) |
| Cl2—C2—C7—O6 | −1.6 (8) | C2—C7—O6—C8 | −170.3 (5) |
| C5—C2—C7—C3 | −2.8 (10) | C6—C8—O6—C7 | −83.3 (7) |
| Cl2—C2—C7—C3 | 177.5 (5) | | |

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O2$^{ii}$ | 0.84 (5) | 2.05 (7) | 2.723 (7) | 136 (8) |
| O1—H1*B*···O2 | 0.84 (3) | 1.82 (5) | 2.619 (7) | 157 (7) |
| O3—H3*A*···O1$^{ii}$ | 0.85 (6) | 2.44 (7) | 3.217 (7) | 153 (7) |
| O3—H3*B*···O6$^{iii}$ | 0.85 (2) | 2.34 (6) | 2.980 (7) | 133 (8) |

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