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Diaquabis(2-carboxybenzoato-κO)-nickel(II)

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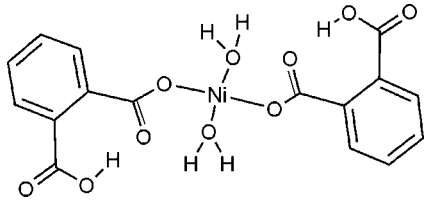
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.090; data-to-parameter ratio = 10.3.

In the title compound, $[Ni(C_8H_5O_4)_2(H_2O)_2]$, the Ni^{II} atom lies on an inversion centre and exhibits a square-planar geometry incorporating two phthalate and two water O atoms. The nickel complex is stabilized by intramolecular interactions involving water O atoms and H atoms of the phthalate groups. It forms one-dimensional zigzag chains along the b axis which are held together *via* π–π stacking interactions (3.647 Å) between the benzene rings of the phthalate groups. The adjacent chains are also hydrogen bonded, resulting in a three-dimensional supramolecular network.

Related literature

For related literature, see: Adiwidjaja & Küppers (1976).



Experimental

Crystal data

$[Ni(C_8H_5O_4)_2(H_2O)_2]$
M_r = 424.98
Monoclinic, $P2_1/c$
a = 8.3601 (17) Å
b = 14.439 (3) Å
c = 7.1005 (14) Å
β = 111.99 (3)°
V = 794.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 291 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS IV diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.784, T_{max} = 0.821
2628 measured reflections
1416 independent reflections
1343 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.07
1416 reflections
137 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5F···O4^{i}	0.86 (2)	1.82 (2)	2.667 (3)	170 (5)
O5—H5E···O3^{ii}	0.86 (2)	1.95 (2)	2.789 (3)	164 (4)
O3—H3E···O2	0.87 (2)	1.54 (2)	2.403 (3)	171 (5)
C2—H2A···O1	0.93	2.33	2.689 (3)	102
C5—H5A···O4	0.93	2.36	2.707 (3)	102

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

Data collection: *R-AXIS* (Rigaku, 1996); cell refinement: *R-AXIS*; data reduction: *R-AXIS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1997); software used to prepare material for publication: *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2050).

References

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supporting information

Acta Cryst. (2008). E**64**, m101 [https://doi.org/10.1107/S1600536807064604]

Diaquabis(2-carboxybenzoato-κO)nickel(II)

Ya-Wen Xuan, Wen Wu, Dong-Po Xie and Nai-Xiang Yuan

S1. Comment

The molecule of the title complex, (I) (Fig. 1), is centrosymmetric, which crystallizes in space group $P2_1/c$. Its structure may be described as one-dimensional zigzag chains (Fig. 2) lying parallel to the b-Axis. It exhibits π-π stacking interactions belonging to a face-to-face form with the distance 3.647 Å. A three dimensional network is thus formed by π-π stacking interaction of phthalates and hydrogen bonds; details of hydrogen-bonding parameters have been provided in the Table.

S2. Experimental

Potassium hydrogen phthalate (0.2040 g, 1 mmol), and KOH (0.0560 g, 1 mmol) were dissolved in 50 ml EtOH/H_2O (V:V = 1:1). To this solution was added a solution of $Ni(NO_3)_2.6H_2O$ (0.2901 g, 1 mmol) in 10 ml double-distilled water. The resulting solution was heated at 373 K for 96 h. After cooling to room temperature, blue crystals suitable for X-ray analysis were obtained in a yield up to 65.42%.

S3. Refinement

H atoms bonded to O atoms were located in a difference map and refined with distance restraints of O—H = 0.85 (1) Å, and with U_{iso}(H) = 1.2Ueq of the parent atoms. Other H atoms were positioned geometrically (C—H = 0.93 Å) and refined in a riding mode with U_{iso}(H) = 1.2Ueq(carrier atoms).

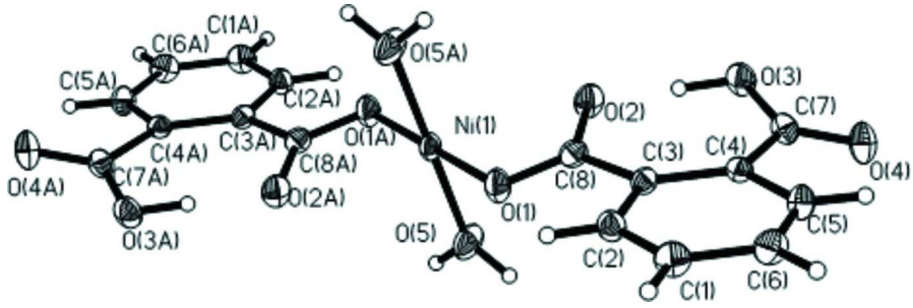

Figure 1

A view of (I) with 30% probability ellipsoid.

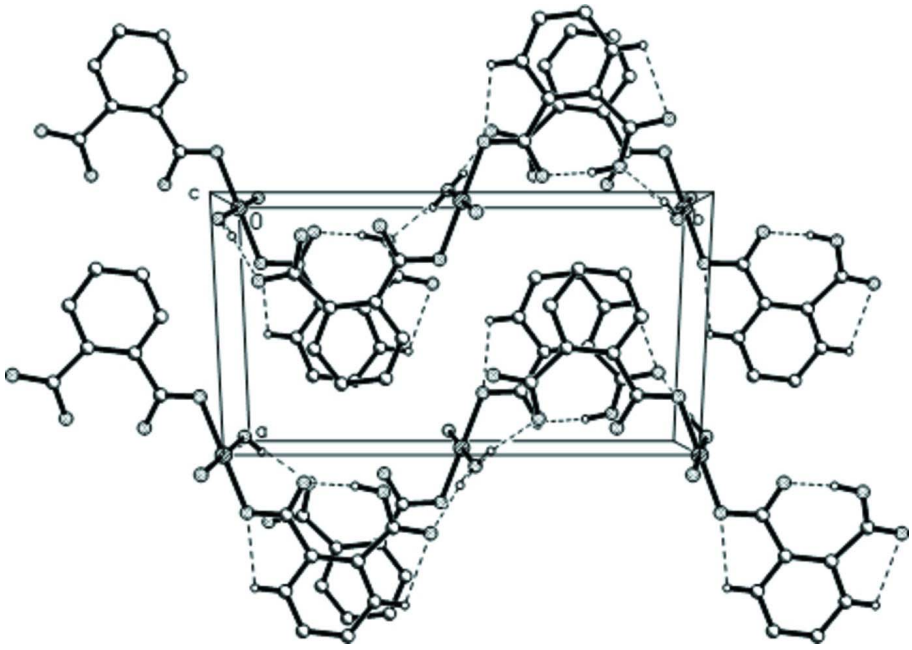

Figure 2

Unit cell packing of (I) showing hydrogen-bonding interactions.

Diaquabis(2-carboxybenzoato-*κO*)nickel(II)

Crystal data

$[Ni(C_8H_5O_4)_2(H_2O)_2]$
M_r = 424.98
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c = 7.1005 (14) Å
β = 111.99 (3)°
V = 794.8 (3) Å^3
Z = 2
$F(000)$ = 436
D_x = 1.776 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 132 reflections
θ = 2–25.1°
μ = 1.28 mm^{-1}
T = 291 K
Block, green
0.20 × 0.18 × 0.16 mm

Data collection

Rigaku R-AXIS-IV diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
Oscillation frames scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.784, T_{max} = 0.821
2628 measured reflections
1416 independent reflections
1343 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.5°, θ_{min} = 2.6°
$h = -10 \rightarrow 9$
$k = -17 \rightarrow 17$
$l = 0 \rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.090
S = 1.07
1416 reflections
137 parameters
3 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

$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2 + 0.5337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.38$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.094 (6)

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}
Ni1	0.0000	0.0000	0.0000	0.0284 (2)
C1	0.7040 (3)	0.16274 (19)	0.2060 (4)	0.0391 (6)
H3A	0.7980	0.1236	0.2300	0.047*
C2	0.5426 (3)	0.12637 (17)	0.1689 (4)	0.0327 (6)
H2A	0.5285	0.0624	0.1650	0.039*
C3	0.3998 (3)	0.18327 (16)	0.1369 (3)	0.0266 (5)
C4	0.4213 (3)	0.28095 (16)	0.1374 (3)	0.0268 (5)
C5	0.5852 (3)	0.31545 (18)	0.1721 (4)	0.0362 (6)
H5A	0.6011	0.3792	0.1715	0.043*
C6	0.7252 (3)	0.25758 (19)	0.2075 (4)	0.0388 (6)
H4A	0.8338	0.2826	0.2323	0.047*
C7	0.2857 (3)	0.35548 (17)	0.1007 (4)	0.0328 (6)
C8	0.2350 (3)	0.13200 (17)	0.0993 (4)	0.0303 (5)
H3E	0.117 (6)	0.2779 (15)	0.110 (7)	0.094 (15)*
H5E	0.006 (4)	0.063 (2)	−0.329 (5)	0.065 (11)*
H5F	−0.132 (5)	−0.003 (2)	−0.378 (5)	0.084 (15)*
O1	0.2296 (2)	0.04720 (12)	0.0575 (3)	0.0388 (5)
O2	0.1034 (2)	0.17147 (13)	0.1107 (3)	0.0417 (5)
O3	0.1404 (2)	0.33670 (13)	0.1202 (3)	0.0416 (5)
O4	0.3147 (3)	0.43396 (12)	0.0568 (3)	0.0461 (5)
O5	−0.0588 (3)	0.02971 (16)	−0.2854 (3)	0.0514 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0268 (3)	0.0215 (3)	0.0385 (3)	−0.00561 (15)	0.0141 (2)	−0.00150 (16)
C1	0.0271 (13)	0.0423 (15)	0.0479 (16)	0.0051 (11)	0.0139 (11)	0.0009 (12)
C2	0.0332 (13)	0.0285 (12)	0.0370 (14)	0.0017 (10)	0.0136 (11)	0.0003 (10)

C3	0.0244 (11)	0.0286 (12)	0.0264 (12)	−0.0023 (9)	0.0091 (9)	0.0009 (9)
C4	0.0285 (12)	0.0278 (12)	0.0244 (11)	−0.0010 (9)	0.0101 (9)	−0.0014 (9)
C5	0.0338 (13)	0.0308 (12)	0.0417 (14)	−0.0072 (10)	0.0117 (11)	−0.0015 (10)
C6	0.0244 (12)	0.0467 (15)	0.0450 (16)	−0.0068 (11)	0.0127 (11)	−0.0037 (12)
C7	0.0322 (13)	0.0288 (13)	0.0327 (13)	0.0002 (10)	0.0068 (10)	−0.0029 (10)
C8	0.0273 (12)	0.0330 (13)	0.0311 (13)	0.0003 (10)	0.0114 (10)	0.0026 (10)
O1	0.0313 (10)	0.0299 (9)	0.0567 (12)	−0.0055 (7)	0.0187 (9)	−0.0027 (8)
O2	0.0301 (9)	0.0381 (10)	0.0631 (13)	−0.0014 (8)	0.0244 (9)	0.0017 (8)
O3	0.0369 (11)	0.0327 (10)	0.0602 (13)	0.0062 (8)	0.0240 (9)	−0.0020 (9)
O4	0.0421 (11)	0.0269 (9)	0.0613 (13)	0.0010 (8)	0.0102 (9)	0.0052 (8)
O5	0.048 (13)	0.0511 (13)	0.0440 (12)	−0.0266 (11)	0.0147 (10)	0.0008 (10)

Geometric parameters (Å, º)

Ni1—O1^{i}	1.9308 (18)	C4—C7	1.513 (3)
Ni1—O1	1.9308 (18)	C5—C6	1.382 (4)
Ni1—O5^{i}	1.946 (2)	C5—H5A	0.9300
Ni1—O5	1.946 (2)	C6—H4A	0.9300
C1—C2	1.378 (4)	C7—O4	1.223 (3)
C1—C6	1.380 (4)	C7—O3	1.302 (3)
C1—H3A	0.9300	C8—O1	1.257 (3)
C2—C3	1.396 (3)	C8—O2	1.268 (3)
C2—H2A	0.9300	O3—H3E	0.87 (2)
C3—C4	1.422 (3)	O5—H5E	0.86 (2)
C3—C8	1.497 (3)	O5—H5F	0.86 (2)
C4—C5	1.391 (3)		
O1^{i}—Ni1—O1	180.00	C6—C5—C4	121.8 (2)
O1^{i}—Ni1—O5^{i}	89.20 (9)	C6—C5—H5A	119.1
O1—Ni1—O5^{i}	90.80 (9)	C4—C5—H5A	119.1
O1^{i}—Ni1—O5	90.80 (9)	C1—C6—C5	120.0 (2)
O1—Ni1—O5	89.20 (9)	C1—C6—H4A	120.0
O5^{i}—Ni1—O5	180.00	C5—C6—H4A	120.0
C2—C1—C6	119.6 (2)	O4—C7—O3	120.1 (2)
C2—C1—H3A	120.2	O4—C7—C4	119.7 (2)
C6—C1—H3A	120.2	O3—C7—C4	120.1 (2)
C1—C2—C3	121.6 (2)	O1—C8—O2	119.8 (2)
C1—C2—H2A	119.2	O1—C8—C3	118.2 (2)
C3—C2—H2A	119.2	O2—C8—C3	121.9 (2)
C2—C3—C4	119.0 (2)	C8—O1—Ni1	109.8 (2)
C2—C3—C8	114.3 (2)	C7—O3—H3E	113 (3)
C4—C3—C8	126.7 (2)	Ni1—O5—H5E	123 (2)
C5—C4—C3	118.1 (2)	Ni1—O5—H5F	120 (3)
C5—C4—C7	113.6 (2)	H5E—O5—H5F	113 (4)
C3—C4—C7	128.3 (2)		
C6—C1—C2—C3	−1.4 (4)	C3—C4—C7—O4	−161.9 (2)
C1—C2—C3—C4	1.7 (4)	C5—C4—C7—O3	−161.5 (2)

C1—C2—C3—C8	−179.9 (2)	C3—C4—C7—O3	19.7 (4)
C2—C3—C4—C5	−0.6 (3)	C2—C3—C8—O1	−14.6 (3)
C8—C3—C4—C5	−178.9 (2)	C4—C3—C8—O1	163.7 (2)
C2—C3—C4—C7	178.1 (2)	C2—C3—C8—O2	164.6 (2)
C8—C3—C4—C7	−0.1 (4)	C4—C3—C8—O2	−17.1 (4)
C3—C4—C5—C6	−0.7 (4)	O2—C8—O1—Ni1	4.3 (3)
C7—C4—C5—C6	−179.6 (2)	C3—C8—O1—Ni1	−176.50 (16)
C2—C1—C6—C5	0.1 (4)	O5^{i}—Ni1—O1—C8	−89.48 (18)
C4—C5—C6—C1	1.0 (4)	O5—Ni1—O1—C8	90.52 (18)
C5—C4—C7—O4	16.9 (3)		

Symmetry code: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*F*···O4^{ii}	0.86 (2)	1.82 (2)	2.667 (3)	170 (5)
O5—H5*E*···O3^{iii}	0.86 (2)	1.95 (2)	2.789 (3)	164 (4)
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Symmetry codes: (ii) −*x*, *y*−1/2, −*z*−1/2; (iii) *x*, −*y*+1/2, *z*−1/2.