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Hexaaquanickel(II) 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate monohydrate

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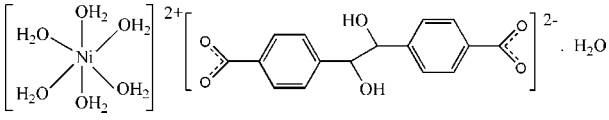
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.071; wR factor = 0.184; data-to-parameter ratio = 14.9.

In the title compound, $[Ni(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$, the Ni^{II} cation is located on a mirror plane and is coordinated by six water molecules, two of which are also located on the mirror plane, in a distorted octahedral geometry. The 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate anion is centrosymmetric with the mid-point of the central ethane C—C bond located on an inversion center. The uncoordinated water molecule is located on a mirror plane. Extensive O—H···O hydrogen bonding is present in the crystal structure.

Related literature

For metal-organic networks constructed from benzene–multicarboxylate ligands, see: Wisser *et al.* (2008); Sun *et al.* (2006); Janiak (2003). For structures incorporating benzene-1,4-dicarboxylate, see: Carton *et al.* (2007); Manna *et al.* (2007); Banerjee *et al.* (2005).



Experimental

Crystal data

$[Ni(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$
M_r = 485.08
Monoclinic, $P2_1/m$
a = 6.0189 (12) Å
b = 20.436 (4) Å
c = 8.6096 (17) Å
β = 103.95 (3)°
V = 1027.8 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.21 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.751, T_{max} = 0.816
9071 measured reflections
2120 independent reflections
2024 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.184
S = 1.03
2120 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H10···O1^{i}	0.89	1.94	2.810 (6)	168
O1W—H1W···O1^{ii}	0.84	1.87	2.684 (5)	162
O2W—H3W···O1	0.84	2.01	2.821 (6)	163
O2W—H4W···O2^{ii}	0.84	1.83	2.667 (6)	174
O3W—H5W···O5W^{iii}	0.84	2.06	2.724 (10)	136
O3W—H6W···O1W^{iv}	0.84	1.98	2.783 (8)	161
O4W—H7W···O5W^{v}	0.84	2.23	3.017 (8)	157
O4W—H8W···O3^{vi}	0.84	2.05	2.840 (6)	157
O5W—H9W···O2	0.84	1.95	2.776 (8)	168

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5046).

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Hexaaquanickel(II) 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate monohydrate

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S1. Comment

Metal-organic networks constructed by benzene-multicarboxylato ligands, have attracted a great deal of recent interest (Wisser *et al.*, 2008; Sun *et al.*, 2006; Janiak *et al.*, 2003). Benzene-1,4-dicarboxylate with a 180° angle between the two carboxylic groups, can form short bridges *via* one carboxylato end and long bridges *via* the benzene ring, leading to a great variety of novel structures (Carton *et al.*, 2007; Manna *et al.*, 2007; Banerjee *et al.*, 2005). Considering that in mind, our group select a derivative of the benzene-1,4-dicarboxylate named 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate to react with $Ni(NO3)_2$ to obtain novel metal-organic complex.

In figure 1, the title compound $(C_{16}H_{12}O_6)[Ni6H_2O].H_2O$ is obtained under hydrothermal condition, which comprises one 4,4′-(1,2-dihydroxyethane-1,2 -diyl)dibenzoate anion, one $[Ni6H_2O]^{2+}$ cation and a solvent water molecule, of which the $[Ni6H_2O]^{2+}$ cation and solvent water is lying on mirror planes, and the anion is locating on an inversion center. the two carboxyl groups of the ligand are total deprotonated, indicated by a difference of the bond lengths, which are also lying in the plane of the benzene rings. and the Ni^{II} center is coordinated by six water molecules instead of the 4,4′-(1,2-dihydroxyethane- 1,2-diyl)dibenzoate ligand. the O—H···O hydrogen bonding interactions between the carboxyl and hydroxyl of the ligands build an infinite chain along *a* axis. the chains, $[Ni6H_2O]^{2+}$ cations and solvent water molecules was further linked by additional O—H···O hydrogen bonds, forming a three-dimensional network.

S2. Experimental

A solution of 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoic acid (0.5 mol, 0.15 g) and $Ni(NO_3)_2$ (0.5 mol, 0.14 g) and 20 ml water was stirred continuously, whose pH was adjusted to 7 by the addition of NaOH solution. The solution was then sealed in an autoclave equipped with a Teflon liner (20 ml) and heated at 373 K for 4 days. Crystals of the title compound were obtained by slow evaporation at room temperature.

S3. Refinement

H atoms bound to C atoms were placed at calculated positions and were treated as riding on the parent atoms with C—H = 0.93 Å (aromatic) and 0.98 Å (CH) and with U_{iso}(H) = 1.2 U_{eq}(C). H atoms of hydroxyl group and water molecules were located in a difference Fourier map and refined as riding with O—H = 0.85+_0.01 Å and U_{iso}(H) = 1.5U_{eq}(O) for water O atoms and O—H = 0.89±0.01 Å and 1.2 U_{eq}(O) for hydroxyl.

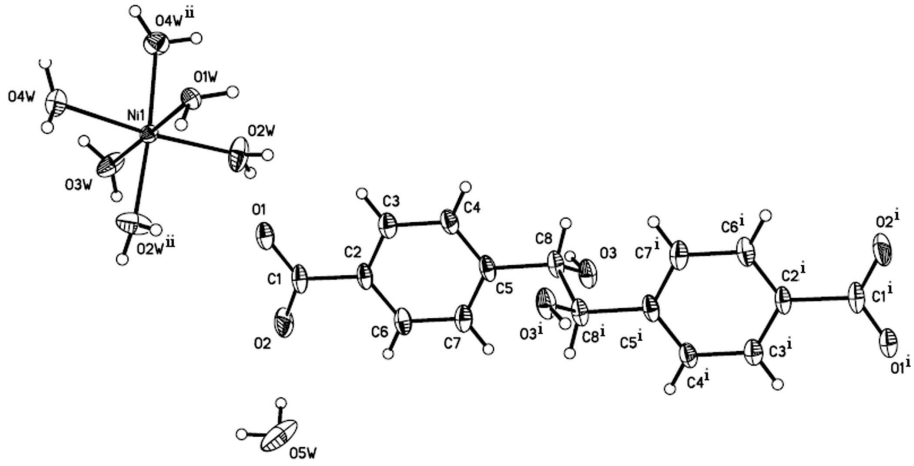

Figure 1

The title compound, with the atom-numbering scheme. Non-H atoms are shown with 30% probability displacement ellipsoids (H atoms are represented by arbitrary spheres). [Symmetry codes: (i) -*x*, -*y*, -*z*; (ii) *x*, 0.5 - *y*, *z*.]

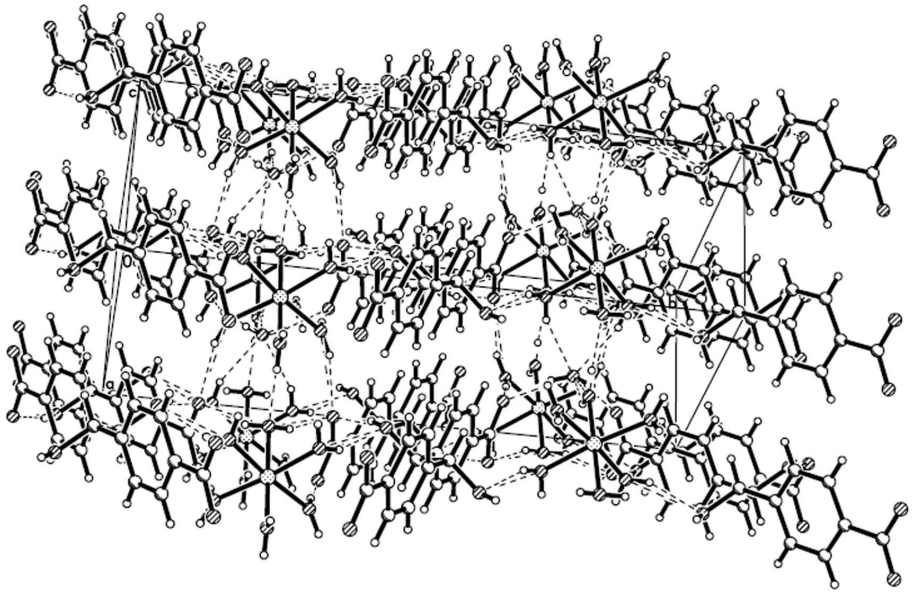

Figure 2

The packing and hydrogen bonding of the title compound.

Hexaaquanickel(II) 4,4′-(1,2-dihydroxyethane-1,2-diyl)dibenzoate monohydrate

Crystal data

$[Ni(H_2O)_6](C_{16}H_{12}O_6)\cdot H_2O$
$M_r = 485.08$
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
$a = 6.0189\ (12)$ Å
$b = 20.436\ (4)$ Å
$c = 8.6096\ (17)$ Å
$\beta = 103.95\ (3)°$
$V = 1027.8\ (4)$ Å^3
$Z = 2$
$F(000) = 508$
$D_x = 1.567$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3600 reflections
$\theta = 1.4–28°$
$\mu = 1.01$ mm^{-1}
$T = 293$ K
Block, green
0.30 × 0.25 × 0.21 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (REQAB; Jacobson, 1998)
T_{min} = 0.751, T_{max} = 0.816
9071 measured reflections
2120 independent reflections
2024 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.2°, θ_{min} = 3.2°
$h = -7 \rightarrow 7$
$k = -25 \rightarrow 25$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.184
S = 1.03
2120 reflections
142 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 10.P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.14235 (16)	0.2500	0.95708 (11)	0.0242 (3)
O1W	−0.2105 (8)	0.2500	0.8578 (6)	0.0279 (11)
H1W	−0.2488	0.2152	0.8065	0.042*
O2W	0.1795 (7)	0.1762 (3)	0.8058 (6)	0.0555 (14)
H3W	0.2947	0.1584	0.7850	0.083*
H4W	0.0631	0.1713	0.7301	0.083*
O3W	0.4872 (10)	0.2500	1.0567 (7)	0.0504 (18)
H5W	0.5246	0.2500	1.1572	0.076*
H6W	0.6021	0.2500	1.0175	0.076*
O4W	0.0917 (8)	0.3180 (2)	1.1214 (5)	0.0439 (11)
H7W	0.0201	0.3101	1.1918	0.066*
H8W	0.0439	0.3509	1.0647	0.066*
O1	0.5811 (7)	0.1431 (2)	0.7095 (5)	0.0438 (11)
O2	0.8274 (7)	0.1532 (3)	0.5570 (6)	0.0559 (14)
O3	0.1710 (8)	−0.0731 (2)	0.0238 (6)	0.0478 (12)
H10	0.2666	−0.0921	0.1056	0.072*

C1	0.6426 (10)	0.1337 (3)	0.5802 (8)	0.0404 (15)
C2	0.4864 (9)	0.0953 (3)	0.4462 (7)	0.0352 (13)
C3	0.2822 (10)	0.0692 (3)	0.4681 (8)	0.0401 (14)
H1	0.2394	0.0765	0.5635	0.048*
C4	0.1421 (10)	0.0323 (3)	0.3473 (7)	0.0397 (14)
H2	0.0051	0.0155	0.3621	0.048*
C5	0.2046 (10)	0.0205 (3)	0.2063 (7)	0.0364 (14)
C6	0.5483 (10)	0.0834 (3)	0.3050 (8)	0.0416 (15)
H4	0.6852	0.1004	0.2903	0.050*
C7	0.4090 (11)	0.0465 (3)	0.1839 (8)	0.0432 (15)
H3	0.4520	0.0392	0.0886	0.052*
C8	0.0514 (10)	−0.0204 (3)	0.0746 (7)	0.0389 (14)
H9	−0.0740	−0.0384	0.1158	0.047*
O5W	0.8270 (14)	0.2500	0.3307 (9)	0.097 (4)
H9W	0.8455	0.2192	0.3971	0.145*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0219 (5)	0.0290 (5)	0.0213 (5)	0.000	0.0045 (3)	0.000
O1W	0.024 (2)	0.026 (3)	0.032 (3)	0.000	0.003 (2)	0.000
O2W	0.028 (2)	0.076 (4)	0.056 (3)	0.008 (2)	−0.003 (2)	−0.036 (3)
O3W	0.027 (3)	0.099 (6)	0.021 (3)	0.000	−0.003 (2)	0.000
O4W	0.048 (2)	0.045 (3)	0.037 (2)	−0.002 (2)	0.0068 (19)	−0.010 (2)
O1	0.036 (2)	0.041 (2)	0.045 (3)	−0.0026 (19)	−0.0069 (19)	−0.011 (2)
O2	0.032 (2)	0.071 (3)	0.058 (3)	−0.013 (2)	−0.002 (2)	−0.027 (3)
O3	0.050 (3)	0.030 (2)	0.052 (3)	0.004 (2)	−0.010 (2)	−0.007 (2)
C1	0.033 (3)	0.033 (3)	0.045 (4)	0.005 (3)	−0.012 (3)	−0.014 (3)
C2	0.029 (3)	0.028 (3)	0.039 (3)	0.003 (2)	−0.010 (2)	−0.009 (2)
C3	0.038 (3)	0.036 (3)	0.040 (3)	−0.001 (3)	−0.003 (3)	−0.006 (3)
C4	0.036 (3)	0.035 (3)	0.041 (3)	−0.007 (3)	−0.006 (3)	−0.003 (3)
C5	0.035 (3)	0.022 (3)	0.041 (3)	0.001 (2)	−0.013 (2)	−0.002 (2)
C6	0.031 (3)	0.039 (3)	0.047 (4)	−0.001 (3)	−0.005 (3)	−0.013 (3)
C7	0.039 (3)	0.041 (3)	0.041 (3)	0.002 (3)	−0.007 (3)	−0.010 (3)
C8	0.036 (3)	0.028 (3)	0.044 (3)	0.000 (2)	−0.009 (3)	−0.008 (3)
O5W	0.062 (5)	0.197 (12)	0.033 (4)	0.000	0.015 (4)	0.000

Geometric parameters (Å, º)

Ni1—O2W^{i}	2.039 (5)	O3—H10	0.8851
Ni1—O2W	2.039 (4)	C1—C2	1.519 (7)
Ni1—O3W	2.046 (6)	C2—C6	1.376 (9)
Ni1—O4W	2.058 (4)	C2—C3	1.393 (9)
Ni1—O4W^{i}	2.058 (4)	C3—C4	1.392 (8)
Ni1—O1W	2.090 (5)	C3—H1	0.9300
O1W—H1W	0.8400	C4—C5	1.377 (9)
O2W—H3W	0.8400	C4—H2	0.9300
O2W—H4W	0.8400	C5—C7	1.395 (9)

O3W—H5W	0.8400	C5—C8	1.526 (7)
O3W—H6W	0.8400	C6—C7	1.393 (8)
O4W—H7W	0.8400	C6—H4	0.9300
O4W—H8W	0.8398	C7—H3	0.9300
O1—C1	1.269 (8)	C8—C8^{ii}	1.531 (12)
O2—C1	1.242 (8)	C8—H9	0.9800
O3—C8	1.422 (7)	O5W—H9W	0.8396

O2W^{i}—Ni1—O2W	95.4 (3)	O2—C1—C2	117.2 (6)
O2W^{i}—Ni1—O3W	90.66 (17)	O1—C1—C2	119.1 (6)
O2W—Ni1—O3W	90.66 (17)	C6—C2—C3	119.2 (5)
O2W^{i}—Ni1—O4W	89.8 (2)	C6—C2—C1	120.8 (6)
O2W—Ni1—O4W	174.6 (2)	C3—C2—C1	120.0 (6)
O3W—Ni1—O4W	90.87 (18)	C4—C3—C2	120.1 (6)
O2W^{i}—Ni1—O4W^{i}	174.6 (2)	C4—C3—H1	119.9
O2W—Ni1—O4W^{i}	89.8 (2)	C2—C3—H1	119.9
O3W—Ni1—O4W^{i}	90.87 (18)	C5—C4—C3	120.5 (6)
O4W—Ni1—O4W^{i}	85.0 (3)	C5—C4—H2	119.7
O2W^{i}—Ni1—O1W	89.75 (16)	C3—C4—H2	119.7
O2W—Ni1—O1W	89.75 (16)	C4—C5—C7	119.5 (5)
O3W—Ni1—O1W	179.4 (2)	C4—C5—C8	120.4 (6)
O4W—Ni1—O1W	88.68 (17)	C7—C5—C8	120.1 (6)
O4W^{i}—Ni1—O1W	88.68 (17)	C2—C6—C7	121.0 (6)
Ni1—O1W—H1W	109.7	C2—C6—H4	119.5
Ni1—O2W—H3W	132.8	C7—C6—H4	119.5
Ni1—O2W—H4W	112.6	C6—C7—C5	119.7 (6)
H3W—O2W—H4W	111.1	C6—C7—H3	120.2
Ni1—O3W—H5W	115.1	C5—C7—H3	120.2
Ni1—O3W—H6W	133.0	O3—C8—C5	112.6 (5)
H5W—O3W—H6W	111.9	O3—C8—C8^{ii}	106.6 (7)
Ni1—O4W—H7W	123.6	C5—C8—C8^{ii}	112.0 (6)
Ni1—O4W—H8W	103.2	O3—C8—H9	108.5
H7W—O4W—H8W	114.1	C5—C8—H9	108.5
C8—O3—H10	111.6	C8^{ii}—C8—H9	108.5
O2—C1—O1	123.7 (5)		

O2—C1—C2—C6	−0.5 (9)	C3—C2—C6—C7	0.7 (9)
O1—C1—C2—C6	−179.2 (6)	C1—C2—C6—C7	177.9 (6)
O2—C1—C2—C3	176.7 (6)	C2—C6—C7—C5	−0.6 (10)
O1—C1—C2—C3	−2.0 (9)	C4—C5—C7—C6	0.6 (9)
C6—C2—C3—C4	−0.7 (9)	C8—C5—C7—C6	−179.6 (5)
C1—C2—C3—C4	−178.0 (6)	C4—C5—C8—O3	−126.7 (6)
C2—C3—C4—C5	0.8 (9)	C7—C5—C8—O3	53.5 (8)
C3—C4—C5—C7	−0.7 (9)	C4—C5—C8—C8^{ii}	113.2 (8)
C3—C4—C5—C8	179.6 (5)	C7—C5—C8—C8^{ii}	−66.6 (9)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H10···O1^{iii}	0.89	1.94	2.810 (6)	168
O1*W*—H1*W*···O1^{iv}	0.84	1.87	2.684 (5)	162
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O2*W*—H4*W*···O2^{iv}	0.84	1.83	2.667 (6)	174
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O4*W*—H7*W*···O5*W*^{vii}	0.84	2.23	3.017 (8)	157
O4*W*—H8*W*···O3^{viii}	0.84	2.05	2.840 (6)	157
O5*W*—H9*W*···O2	0.84	1.95	2.776 (8)	168

Symmetry codes: (iii) −*x*+1, −*y*, −*z*+1; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*+1; (vi) *x*+1, *y*, *z*; (vii) *x*−1, *y*, *z*+1; (viii) −*x*, *y*+1/2, −*z*+1.