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Hexaaquanickel(II) chelidonate monohydrate

Vaduganathan Yasodha,[a] Subbaiah Govindarajan,[a]* V. Manivannan[b] and O. Büyükgüngör[c]

[a]Department of Chemistry, Bharathiar University, Coimbatore 641 046, India, [b]Department of Physics, Presidency College, Chennai 600 005, India, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Samsun, Turkey
Correspondence e-mail: drsgovind@rediffmail.com

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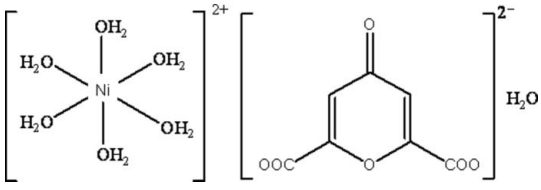
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.023; wR factor = 0.056; data-to-parameter ratio = 14.9.

In the title hydrated molecular salt, $[Ni(H_2O)_6](C_7H_2O_6)\cdot H_2O$, the Ni cation adopts a slightly distorted octahedral geometry. In the crystal structure, the component species interact by way of O—H···O and weak C—H···O interactions, resulting in a three-dimensional network.

Related literature

For background, see: Manojlovic-Muir *et al.* (1999); Qu *et al.* (2004); Yasodha *et al.* (2007).



Experimental

Crystal data

$[Ni(H_2O)_6](C_7H_2O_6)\cdot H_2O$
M_r = 366.91
Monoclinic, $P2_1/n$
a = 6.9471 (4) Å
b = 17.3603 (8) Å
c = 11.6372 (6) Å
β = 104.884 (4)°
V = 1356.40 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.50 mm^{-1}
T = 150 (2) K
0.53 × 0.46 × 0.37 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.504, T_{max} = 0.607
24142 measured reflections
3772 independent reflections
3508 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.057
S = 1.06
3772 reflections
254 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O7	2.0253 (9)	Ni1—O8	2.0524 (9)
Ni1—O10	2.0304 (9)	Ni1—O9	2.0617 (9)
Ni1—O11	2.0460 (9)	Ni1—O12	2.0894 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O1^{i}	0.84 (2)	2.49 (2)	2.9284 (12)	113.4 (18)
O7—H7A···O3^{i}	0.84 (2)	1.85 (2)	2.6862 (13)	174 (2)
O7—H7B···O1^{i}	0.83 (2)	2.55 (2)	2.9284 (12)	109.2 (17)
O7—H7B···O5^{i}	0.83 (2)	1.89 (2)	2.7161 (13)	175 (2)
O8—H8A···O2^{ii}	0.84 (2)	2.01 (2)	2.8281 (13)	165 (2)
O8—H8B···O4^{iii}	0.81 (2)	1.86 (2)	2.6635 (12)	172 (2)
O9—H9A···O2^{iv}	0.82 (2)	2.11 (2)	2.8837 (13)	157 (2)
O9—H9B···O6	0.88 (2)	1.80 (2)	2.6841 (13)	175 (2)
O10—H10A···O4^{v}	0.87 (2)	1.88 (2)	2.7482 (13)	175 (2)
O10—H10B···O5	0.82 (2)	1.98 (2)	2.7980 (14)	169 (2)
O11—H11A···O2^{iv}	0.81 (2)	1.94 (2)	2.7439 (14)	167 (2)
O11—H11B···O13W^{vi}	0.82 (2)	1.90 (2)	2.6738 (14)	157 (2)
O12—H12A···O13W^{ii}	0.90 (2)	2.07 (2)	2.9553 (14)	171 (2)
O12—H12B···O3^{v}	0.85 (2)	1.87 (2)	2.7053 (13)	169 (2)
O13W—H13A···O12^{vii}	0.87 (3)	2.00 (3)	2.8291 (14)	160 (3)
O13W—H13B···O6	0.84 (3)	1.95 (3)	2.7835 (14)	176 (3)
C2—H2···O13W	0.929 (18)	2.591 (19)	3.4755 (16)	159.1 (16)
C4—H4···O8^{iii}	0.958 (18)	2.582 (18)	3.4046 (15)	144.1 (16)

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+2, -y+1, -z+2$; (iv) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{5}{2}$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (vii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); 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: HB2530).

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  doi:10.1107/S1600536807049045

supplementary materials

Acta Cryst. (2007). E**63**, m2720 [**doi:10.1107/S1600536807049045**]

Hexaaquanickel(II) chelidonate monohydrate

V. Yasodha, S. Govindarajan, V. Manivannan and O. Büyükgüngör

Comment

Recently, we reported (Yasodha *et al.*, 2007) a copper complex of the chelidonate (2,6-dicarboxypyranone) dianion arisng from doubly deprotonated 4-pyrone-2,6-dicarboxylic acid in which all the carboxylate oxygen atoms are involved in metal coordination to form a one dimensional polymeric chain. Conversely, in pentaaqua chelidonate copper (II) monohydrate (Manojlovic-Muir *et al.*, 1999), only the carbonyl oxygen atom coordinates to the metal.

As an extension of these studies, we now describe the title compound, (I), which is a hydrated molecular salt (Fig. 1), in which the chelidonate is present as an isolated dianion. The carboxylate groups O5/C6/O6 and O3/C7/O4 form dihedral angles of 7.5 (5)° and 8.51 (8)° with the pyrone ring. The $[Ni(H_2O)_6]^{2+}$ complex cation in (I) adopts a distorted octahedral cooordination, with the axial bonds to O9 and O12 slightly longer than the other four Ni—O vertices (Table 1). The Ni—O distances in (I) are shorter than the distances observed in hexaaquanickel (II) bis(*p*-nitrobenzoate) dihydrate [Ni—O mean distance 2.117 (3) Å] (Qu *et al.*, 2004).

In the crystal a network of O—H···O and possible C—H···O interactions (Table 2, Fig. 2) help to establish the packing in which chains of chelidonate moieties form chains mediated by the complex cations.

Experimental

An aqueous mixture of $Ni(OH)_2Ni(CO_3)_24H_2O$ and chelidonic acid in a 1:1 molar ratio yielded dark green blocks of (I) after 15 days, which were washed with ice cold water and dried in air (yield 55%). Elemental analysis found (calc)%: C 23.1 (22.9) H 4.38 (4.40). The % metal content was determined experimentally by complexometric edta titration as 15.88 (16.00).

Refinement

H atoms bonded to O and C atoms were located in a difference map and refined with distance restraints of O—H = 0.82 (2)–0.92 (2) Å and with U_{iso}(H) = 1.2Ueq(O) and C—H = 0.92 (2)–0.97 (2) Å and with U_{iso}(H) = 1.2Ueq(C).

Figures

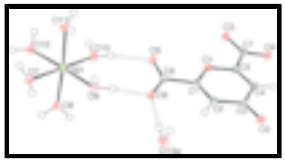

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. The hydrogen bonds are indicated by double dashed lines.

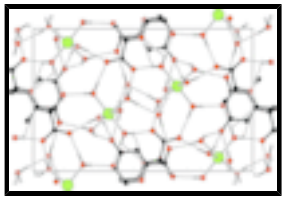

Fig. 2. The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Hexaaquanickel(II) chelidonate monohydrate

Crystal data

$[Ni(H_2O)_6](C_7H_2O_6)\cdot H_2O$	F_{000} = 760
	D_x = 1.797 Mg m^{-3}
M_r = 366.91	D_m = 1.80 Mg m^{-3}
	D_m measured by not measured
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
	λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 24142 reflections
a = 6.9471 (4) Å	θ = 1.8–29.6º
b = 17.3603 (8) Å	μ = 1.50 mm^{-1}
c = 11.6372 (6) Å	T = 150 (2) K
β = 104.884 (4)º	Block, green
V = 1356.40 (12) Å^3	0.53 × 0.46 × 0.37 mm
Z = 4	

Data collection

Stoe IPDSII diffractometer	3772 independent reflections
Radiation source: fine-focus sealed tube	3508 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.026
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 29.5º
T = 150(2) K	θ_{min} = 2.2º
rotation method scans	h = −9→9
Absorption correction: integration (X-RED; Stoe & Cie, 2002)	k = −24→21
T_{min} = 0.504, T_{max} = 0.607	l = −16→16
24142 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.023	All H-atom parameters refined
$wR(F^2)$ = 0.057	$w = 1/[\sigma^2(F_o^2) + (0.028P)^2 + 0.7192P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$

3772 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
254 parameters	$\Delta\rho_{min} = -0.52$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.83531 (2)	0.156381 (8)	0.903233 (13)	0.01138 (5)
O7	0.73282 (13)	0.08375 (5)	0.76483 (8)	0.01506 (16)
O8	0.55224 (13)	0.19962 (5)	0.87631 (8)	0.01541 (16)
O1	1.28294 (12)	0.50673 (5)	1.06212 (7)	0.01258 (15)
O4	1.51202 (15)	0.66431 (5)	1.23257 (8)	0.01940 (18)
O12	0.76261 (13)	0.07105 (5)	1.01155 (8)	0.01493 (16)
O10	0.92919 (15)	0.22779 (6)	1.04475 (8)	0.01868 (18)
O11	1.10798 (13)	0.10517 (6)	0.92698 (9)	0.01829 (18)
O5	1.13809 (14)	0.36466 (5)	1.03685 (8)	0.01914 (18)
O9	0.90234 (14)	0.23487 (5)	0.78630 (8)	0.01687 (17)
O6	1.01691 (14)	0.38086 (5)	0.84128 (8)	0.01823 (17)
O3	1.45597 (14)	0.54427 (5)	1.28379 (8)	0.01867 (18)
O2	1.29913 (13)	0.64282 (5)	0.78142 (8)	0.01634 (17)
C6	1.11182 (17)	0.40194 (7)	0.94290 (10)	0.0133 (2)
C7	1.45038 (17)	0.59708 (7)	1.21020 (10)	0.0132 (2)
C3	1.29363 (16)	0.60099 (7)	0.86831 (10)	0.0128 (2)
C2	1.20278 (17)	0.52589 (7)	0.85394 (10)	0.0132 (2)
C1	1.20133 (16)	0.48242 (6)	0.94934 (10)	0.0121 (2)
C5	1.36657 (16)	0.57785 (6)	1.07966 (10)	0.0118 (2)
C4	1.37612 (17)	0.62476 (7)	0.98924 (10)	0.0132 (2)
O13W	0.92491 (14)	0.42877 (6)	0.60517 (9)	0.02049 (19)
H2	1.147 (3)	0.5086 (10)	0.7770 (16)	0.021 (4)*
H4	1.438 (3)	0.6743 (10)	1.0046 (16)	0.022 (4)*
H8A	0.459 (3)	0.1746 (13)	0.832 (2)	0.038 (5)*
H8B	0.542 (3)	0.2423 (14)	0.848 (2)	0.041 (6)*
H12A	0.717 (3)	0.0277 (14)	0.972 (2)	0.046 (6)*
H7A	0.800 (3)	0.0434 (13)	0.765 (2)	0.040 (6)*
H10A	0.956 (3)	0.2080 (14)	1.116 (2)	0.047 (6)*
H11A	1.151 (3)	0.1121 (12)	0.869 (2)	0.038 (5)*
H12B	0.859 (3)	0.0595 (12)	1.070 (2)	0.037 (5)*
H11B	1.201 (3)	0.1070 (12)	0.987 (2)	0.039 (6)*
H9A	0.985 (3)	0.2188 (12)	0.7533 (19)	0.033 (5)*
H10B	1.004 (3)	0.2645 (14)	1.044 (2)	0.043 (6)*
H7B	0.711 (3)	0.1000 (12)	0.696 (2)	0.037 (5)*
H9B	0.944 (3)	0.2819 (14)	0.809 (2)	0.043 (6)*
H13A	1.034 (4)	0.4180 (16)	0.585 (2)	0.068 (8)*
H13B	0.947 (4)	0.4145 (15)	0.676 (3)	0.060 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01381 (8)	0.01007 (8)	0.00988 (8)	−0.00031 (5)	0.00237 (5)	0.00005 (5)
O7	0.0202 (4)	0.0127 (4)	0.0112 (4)	0.0016 (3)	0.0020 (3)	−0.0015 (3)
O8	0.0159 (4)	0.0124 (4)	0.0167 (4)	0.0008 (3)	0.0021 (3)	−0.0002 (3)
O1	0.0161 (4)	0.0107 (4)	0.0104 (4)	−0.0015 (3)	0.0024 (3)	−0.0007 (3)
O4	0.0297 (5)	0.0121 (4)	0.0137 (4)	−0.0031 (3)	0.0006 (3)	−0.0009 (3)
O12	0.0180 (4)	0.0133 (4)	0.0129 (4)	−0.0010 (3)	0.0028 (3)	0.0023 (3)
O10	0.0277 (5)	0.0151 (4)	0.0120 (4)	−0.0066 (3)	0.0029 (3)	−0.0013 (3)
O11	0.0154 (4)	0.0246 (5)	0.0141 (4)	0.0032 (3)	0.0025 (3)	0.0021 (4)
O5	0.0280 (5)	0.0143 (4)	0.0139 (4)	−0.0056 (3)	0.0032 (3)	0.0010 (3)
O9	0.0237 (4)	0.0119 (4)	0.0170 (4)	−0.0013 (3)	0.0088 (3)	0.0003 (3)
O6	0.0249 (4)	0.0150 (4)	0.0131 (4)	−0.0046 (3)	0.0018 (3)	−0.0019 (3)
O3	0.0264 (4)	0.0148 (4)	0.0122 (4)	−0.0043 (3)	0.0004 (3)	0.0019 (3)
O2	0.0205 (4)	0.0156 (4)	0.0130 (4)	−0.0009 (3)	0.0045 (3)	0.0036 (3)
C6	0.0147 (5)	0.0115 (5)	0.0138 (5)	−0.0004 (4)	0.0040 (4)	−0.0013 (4)
C7	0.0152 (5)	0.0127 (5)	0.0111 (5)	0.0005 (4)	0.0021 (4)	−0.0005 (4)
C3	0.0132 (4)	0.0127 (5)	0.0127 (5)	0.0015 (4)	0.0037 (4)	0.0010 (4)
C2	0.0146 (5)	0.0131 (5)	0.0116 (5)	0.0002 (4)	0.0024 (4)	−0.0012 (4)
C1	0.0122 (4)	0.0118 (5)	0.0118 (5)	0.0007 (4)	0.0024 (4)	−0.0016 (4)
C5	0.0123 (4)	0.0099 (5)	0.0127 (5)	0.0005 (4)	0.0023 (4)	−0.0008 (4)
C4	0.0146 (5)	0.0116 (5)	0.0132 (5)	−0.0004 (4)	0.0031 (4)	−0.0007 (4)
O13W	0.0180 (4)	0.0287 (5)	0.0143 (4)	−0.0006 (4)	0.0034 (3)	0.0000 (4)

Geometric parameters (Å, °)

Ni1—O7	2.0253 (9)	O11—H11B	0.82 (2)
Ni1—O10	2.0304 (9)	O5—C6	1.2431 (15)
Ni1—O11	2.0460 (9)	O9—H9A	0.82 (2)
Ni1—O8	2.0524 (9)	O9—H9B	0.88 (2)
Ni1—O9	2.0617 (9)	O6—C6	1.2516 (14)
Ni1—O12	2.0894 (9)	O3—C7	1.2482 (14)
O7—H7A	0.84 (2)	O2—C3	1.2536 (14)
O7—H7B	0.82 (2)	C6—C1	1.5233 (16)
O8—H8A	0.84 (2)	C7—C5	1.5178 (15)
O8—H8B	0.81 (2)	C3—C4	1.4370 (16)
O1—C1	1.3563 (13)	C3—C2	1.4393 (16)
O1—C5	1.3574 (13)	C2—C1	1.3446 (16)
O4—C7	1.2474 (14)	C2—H2	0.928 (18)
O12—H12A	0.90 (2)	C5—C4	1.3457 (16)
O12—H12B	0.84 (2)	C4—H4	0.957 (18)
O10—H10A	0.87 (2)	O13W—H13A	0.87 (3)
O10—H10B	0.82 (2)	O13W—H13B	0.84 (3)
O11—H11A	0.82 (2)		
O7—Ni1—O10	177.73 (4)	Ni1—O11—H11A	110.5 (15)
O7—Ni1—O11	87.77 (4)	Ni1—O11—H11B	126.7 (15)

O10—Ni1—O11	93.58 (4)	H11A—O11—H11B	109 (2)
O7—Ni1—O8	88.79 (4)	Ni1—O9—H9A	113.0 (14)
O10—Ni1—O8	89.78 (4)	Ni1—O9—H9B	122.0 (15)
O11—Ni1—O8	175.64 (4)	H9A—O9—H9B	104 (2)
O7—Ni1—O9	88.82 (4)	O5—C6—O6	126.97 (11)
O10—Ni1—O9	92.97 (4)	O5—C6—C1	117.93 (10)
O11—Ni1—O9	91.03 (4)	O6—C6—C1	115.09 (10)
O8—Ni1—O9	91.58 (4)	O4—C7—O3	126.55 (11)
O7—Ni1—O12	87.03 (4)	O4—C7—C5	115.94 (10)
O10—Ni1—O12	91.18 (4)	O3—C7—C5	117.48 (10)
O11—Ni1—O12	88.24 (4)	O2—C3—C4	122.44 (11)
O8—Ni1—O12	88.90 (4)	O2—C3—C2	122.30 (11)
O9—Ni1—O12	175.82 (4)	C4—C3—C2	115.25 (10)
Ni1—O7—H7A	115.9 (15)	C1—C2—C3	120.56 (11)
Ni1—O7—H7B	119.8 (15)	C1—C2—H2	121.7 (11)
H7A—O7—H7B	104 (2)	C3—C2—H2	117.7 (11)
Ni1—O8—H8A	117.5 (15)	C2—C1—O1	122.31 (10)
Ni1—O8—H8B	112.3 (15)	C2—C1—C6	124.31 (10)
H8A—O8—H8B	104 (2)	O1—C1—C6	113.38 (9)
C1—O1—C5	119.00 (9)	C4—C5—O1	122.55 (10)
Ni1—O12—H12A	113.2 (15)	C4—C5—C7	124.49 (10)
Ni1—O12—H12B	112.9 (15)	O1—C5—C7	112.95 (9)
H12A—O12—H12B	108 (2)	C5—C4—C3	120.31 (11)
Ni1—O10—H10A	118.4 (16)	C5—C4—H4	120.5 (11)
Ni1—O10—H10B	122.3 (16)	C3—C4—H4	119.2 (11)
H10A—O10—H10B	110 (2)	H13A—O13W—H13B	105 (2)
O2—C3—C2—C1	179.43 (11)	C1—O1—C5—C4	−1.62 (16)
C4—C3—C2—C1	−1.02 (16)	C1—O1—C5—C7	179.67 (9)
C3—C2—C1—O1	0.35 (17)	O4—C7—C5—C4	7.95 (17)
C3—C2—C1—C6	−179.01 (10)	O3—C7—C5—C4	−170.19 (11)
C5—O1—C1—C2	0.98 (16)	O4—C7—C5—O1	−173.37 (10)
C5—O1—C1—C6	−179.60 (9)	O3—C7—C5—O1	8.49 (15)
O5—C6—C1—C2	172.73 (11)	O1—C5—C4—C3	0.91 (17)
O6—C6—C1—C2	−7.79 (16)	C7—C5—C4—C3	179.46 (10)
O5—C6—C1—O1	−6.67 (15)	O2—C3—C4—C5	179.96 (11)
O6—C6—C1—O1	172.80 (10)	C2—C3—C4—C5	0.41 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7A···O1^{i}	0.84 (2)	2.49 (2)	2.9284 (12)	113.4 (18)
O7—H7A···O3^{i}	0.84 (2)	1.85 (2)	2.6862 (13)	174 (2)
O7—H7B···O1^{i}	0.83 (2)	2.55 (2)	2.9284 (12)	109.2 (17)
O7—H7B···O5^{i}	0.83 (2)	1.89 (2)	2.7161 (13)	175 (2)
O8—H8A···O2^{ii}	0.84 (2)	2.01 (2)	2.8281 (13)	165 (2)
O8—H8B···O4^{iii}	0.81 (2)	1.86 (2)	2.6635 (12)	172 (2)
O9—H9A···O2^{iv}	0.82 (2)	2.11 (2)	2.8837 (13)	157 (2)

O9—H9B···O6	0.88 (2)	1.80 (2)	2.6841 (13)	175 (2)
O10—H10A···O4^{v}	0.87 (2)	1.88 (2)	2.7482 (13)	175 (2)
O10—H10B···O5	0.82 (2)	1.98 (2)	2.7980 (14)	169 (2)
O11—H11A···O2^{iv}	0.81 (2)	1.94 (2)	2.7439 (14)	167 (2)
O11—H11B···O13W^{vi}	0.82 (2)	1.90 (2)	2.6738 (14)	157 (2)
O12—H12A···O13W^{ii}	0.90 (2)	2.07 (2)	2.9553 (14)	171 (2)
O12—H12B···O3^{v}	0.85 (2)	1.87 (2)	2.7053 (13)	169 (2)
O13W—H13A···O12^{vii}	0.87 (3)	2.00 (3)	2.8291 (14)	160 (3)
O13W—H13B···O6	0.84 (3)	1.95 (3)	2.7835 (14)	176 (3)
C2—H2···O13W	0.929 (18)	2.591 (19)	3.4755 (16)	159.1 (16)
C4—H4···O8^{iii}	0.958 (18)	2.582 (18)	3.4046 (15)	144.1 (16)

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iii) −*x*+2, −*y*+1, −*z*+2; (iv) −*x*+5/2, *y*−1/2, −*z*+3/2; (v) −*x*+5/2, *y*−1/2, −*z*+5/2; (vi) *x*+1/2, −*y*+1/2, *z*+1/2; (vii) *x*+1/2, −*y*+1/2, *z*−1/2.

Fig. 1

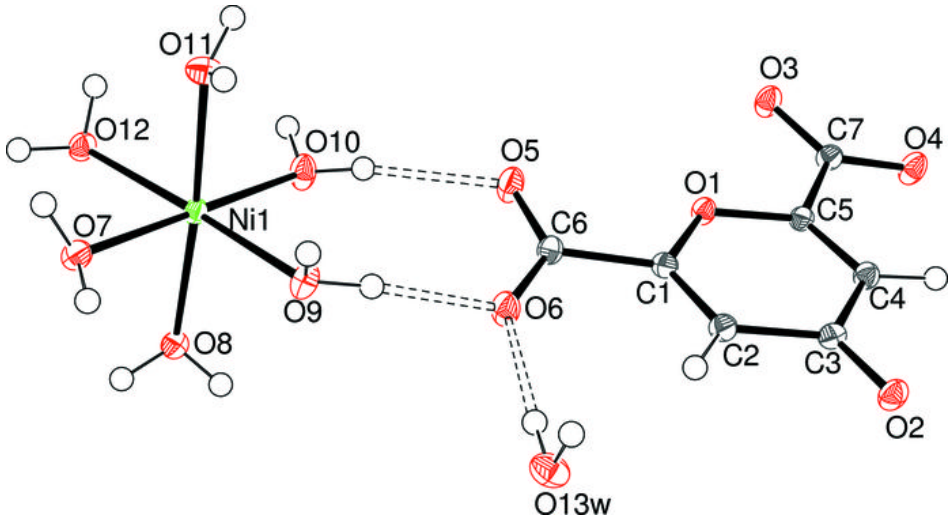

Fig. 2