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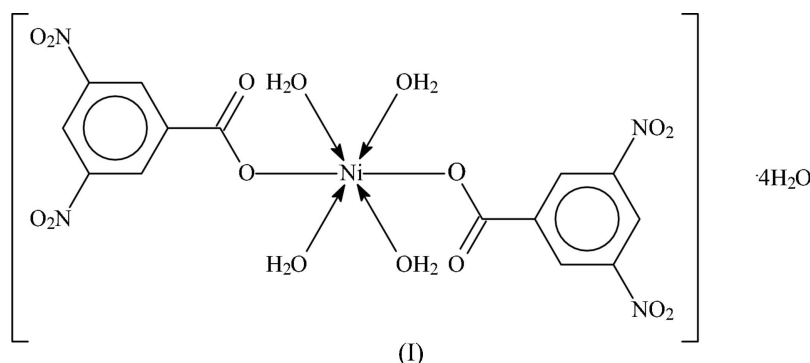
Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.033
 wR factor = 0.097
Data-to-parameter ratio = 13.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Tetraaquabis(3,5-dinitrobenzoato- κ O)nickel(II)
tetrahydrateThe Ni atom in the title compound, $[\text{Ni}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$, is covalently bonded to two dinitrobenzoate groups and datively bonded by four water molecules in a *trans* octahedral geometry; adjacent molecules are linked through the uncoordinated water molecules into a three-dimensional network.

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Comment

The title Ni compound, (I) (Fig. 1), is isostructural with $[\text{Co}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$ (Tahir *et al.*, 1996), whose metal atom is covalently bonded to two dinitrobenzoate groups and datively bonded by four water molecules in a *trans* octahedral geometry. In the Ni compound, the metal-bearing molecule and the uncoordinated water molecules engage in hydrogen bonding (Table 2) to furnish a three-dimensional network. Some spectroscopic and TGA measurements for the title compound have been previously reported (Ferenc, 1995; Odunola *et al.*, 1992).

Experimental

Nickel acetate tetrahydrate (0.124 g, 0.5 mmol) and sodium hydroxide (0.04 g, 1 mmol) were added to an aqueous solution of 3,5-dinitrobenzoic acid (0.212 g, 1 mmol). The solution was filtered and set aside for several days, leading to the formation of green prismatic crystals. Analysis calculated for $\text{C}_{14}\text{H}_{22}\text{N}_4\text{NiO}_{20}$: C 26.90, H 3.55, N 8.96%; found: C 26.85, H 3.49, N 8.99%.

Crystal data

 $[\text{Ni}(\text{C}_7\text{H}_3\text{N}_2\text{O}_6)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$
 $M_r = 625.07$
 Triclinic, $P\bar{1}$
 $a = 7.1835$ (2) Å
 $b = 11.7581$ (3) Å
 $c = 15.0077$ (4) Å
 $\alpha = 103.199$ (1)°
 $\beta = 98.267$ (1)°
 $\gamma = 92.672$ (1)°

 $V = 1217.15$ (6) Å³
 $Z = 2$
 $D_x = 1.706$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.90$ mm⁻¹
 $T = 295$ (2) K
 Prism, green
 $0.36 \times 0.25 \times 0.18$ mm

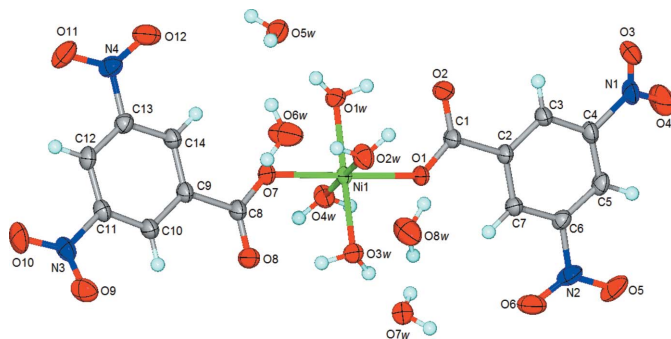


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii.

Data collection

Rigaku R-Axis RAPID IP diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.519$, $T_{\max} = 0.855$

12071 measured reflections
 5527 independent reflections
 4813 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.097$
 $S = 1.06$
 5527 reflections
 416 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.1168P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.36 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.67 \text{ e } \text{\AA}^{-3}$

Table 1
Selected geometric parameters (\AA , $^\circ$).

Ni1—O1	2.022 (1)	Ni1—O2w	2.081 (1)
Ni1—O7	2.017 (1)	Ni1—O3w	2.064 (1)
Ni1—O1w	2.063 (1)	Ni1—O4w	2.090 (1)
O1—Ni1—O7	178.43 (5)	O7—Ni1—O1w	87.07 (5)
O1—Ni1—O1w	91.82 (5)	O7—Ni1—O2w	89.89 (5)
O1—Ni1—O2w	91.28 (5)	O7—Ni1—O3w	93.54 (5)
O1—Ni1—O3w	87.58 (5)	O7—Ni1—O4w	89.84 (5)
O1—Ni1—O4w	89.01 (5)		

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1w—H1w1 \cdots O2	0.85 (1)	1.96 (1)	2.749 (2)	156 (2)
O1w—H1w2 \cdots O5w ⁱ	0.85 (1)	1.91 (1)	2.752 (2)	175 (2)
O2w—H2w1 \cdots O5w ⁱ	0.85 (1)	1.95 (9)	2.801 (2)	177 (3)
O2w—H2w2 \cdots O6w	0.85 (1)	1.88 (1)	2.718 (2)	170 (3)
O3w—H3w1 \cdots O8	0.85 (1)	1.88 (1)	2.692 (2)	159 (2)
O3w—H3w2 \cdots O7w	0.85 (1)	1.96 (1)	2.806 (2)	174 (2)
O4w—H4w1 \cdots O7w ⁱⁱ	0.85 (1)	1.93 (1)	2.784 (2)	175 (2)
O4w—H4w2 \cdots O8w	0.85 (1)	1.98 (1)	2.830 (2)	177 (2)
O5w—H5w1 \cdots O2 ⁱ	0.84 (1)	2.14 (2)	2.894 (2)	148 (3)
O5w—H5w2 \cdots O4w ⁱⁱⁱ	0.84 (1)	2.18 (1)	2.967 (2)	155 (2)
O6w—H6w1 \cdots O2 ⁱ	0.84 (1)	2.04 (2)	2.786 (2)	148 (2)
O7w—H7w2 \cdots O2w ^{iv}	0.84 (1)	2.23 (1)	3.004 (2)	154 (2)
O7w—H7w1 \cdots O8w	0.84 (1)	2.18 (1)	2.999 (2)	163 (2)
O8w—H8w1 \cdots O8 ⁱⁱ	0.85 (1)	1.96 (1)	2.729 (2)	151 (2)

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

The C-bound H atoms were positioned geometrically ($C-H = 0.93 \text{ \AA}$) and were included in the refinement in the riding-model approximation, with $U_{\text{iso}}(H)$ set to $1.2U_{\text{eq}}(C)$. The water H atoms were located in a difference Fourier map, and were refined with a distance restraint of $O-H = 0.85 (1) \text{ \AA}$; their displacement parameters were freely refined.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); method used to solve structure: atomic coordinates taken from the isostructural Co analog (Tahir *et al.*, 1996); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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