

Tetraaquadimidazolenickel(II) naphthalene-1,5-disulfonate

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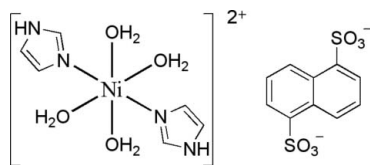
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Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.024; wR factor = 0.067; data-to-parameter ratio = 15.0.

The triclinic unit cell of the title compound, $[\text{Ni}(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_4](\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)$, contains one centrosymmetric cation and one centrosymmetric anion. In the cation, the Ni^{II} ion is six-coordinated by two imidazole ligands [$\text{Ni}-\text{N} = 2.0568$ (14) Å] and four water molecules [both independent $\text{Ni}-\text{O}$ distances are 2.098 (1) Å] in a distorted octahedral geometry. Intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds form an extensive three-dimensional network, which consolidates the crystal packing.

Related literature

For related literature, see: Côté & Shimizu (2003); Cai (2004); Cai *et al.* (2001); Chen *et al.* (2001, 2002); Lian *et al.* (2007); Liu *et al.* (2006); Zhou *et al.* (2004).



Experimental

Crystal data

$[\text{Ni}(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_4](\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)$ $\gamma = 111.967$ (5)°
 $M_r = 553.21$ $V = 554.6$ (3) Å³
 Triclinic, $P\bar{1}$ $Z = 1$
 $a = 8.285$ (3) Å Mo $K\alpha$ radiation
 $b = 8.925$ (3) Å $\mu = 1.12$ mm⁻¹
 $c = 9.088$ (3) Å $T = 273$ (2) K
 $\alpha = 107.705$ (5)° $0.37 \times 0.28 \times 0.22$ mm
 $\beta = 101.628$ (5)°

Data collection

Bruker SMART 1K CCD 4834 measured reflections
 diffractometer 2499 independent reflections
 Absorption correction: multi-scan 2262 reflections with $I > 2\sigma(I)$
 (SADABS; Bruker, 2001) $R_{\text{int}} = 0.011$
 $T_{\text{min}} = 0.681$, $T_{\text{max}} = 0.790$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$ H atoms treated by a mixture of
 $wR(F^2) = 0.067$ independent and constrained
 $S = 1.08$ refinement
 2499 reflections $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 167 parameters $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³
 6 restraints

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1W}-\text{H1WA}\cdots\text{O3}^{\text{i}}$	0.82 (2)	2.022 (15)	2.7507 (18)	148 (2)
$\text{O1W}-\text{H1WB}\cdots\text{O1}$	0.82 (2)	2.018 (14)	2.788 (2)	156 (3)
$\text{O2W}-\text{H2WA}\cdots\text{O1}^{\text{ii}}$	0.81 (2)	1.962 (10)	2.7496 (19)	161 (2)
$\text{O2W}-\text{H2WB}\cdots\text{O2}^{\text{iii}}$	0.81 (2)	1.96 (2)	2.7979 (18)	173 (2)
$\text{N2}-\text{H7A}\cdots\text{O3}^{\text{iv}}$	0.86	2.19	2.981 (2)	154

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); 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: CV2373).

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supplementary materials

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P. Liu and D.-S. Deng

Comment

The weak coordination nature of SO_3^- makes its coordination mode very flexible and sensitive to the chemical environment (Côté *et al.*, 2003). It is known that the coordination behavior of arenesulfonates with transition metals can be tailored in the presence of amino ligands (Lian *et al.*, 2007; Liu *et al.*, 2006; Zhou *et al.*, 2004; Chen *et al.*, 2001; Cai *et al.*, 2001; Chen *et al.*, 2002). Herewith we present the crystal structure of the title compound, $[\text{C}_6\text{H}_{16}\text{N}_4\text{NiO}_4]^{2+} \cdot [\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2]^{2-}$ (I) (Fig. 1).

The asymmetric unit of (I) contains a half of complex cation and a half of organic anion. Four water molecules coordinate to the nickel ion in *trans* position, respectively, and two imine nitrogen atoms from two imidazole ligands coordinate to nickel atom in *trans* position too. Thus, the nickel ion has a slightly distorted octahedral coordination geometry.

The title compound adopts the same hybrid organic-inorganic packing pattern as that reported earlier (Cai, 2004; Chen *et al.*, 2001; Cai *et al.*, 2001; Chen *et al.*, 2002). The intermolecular O—H \cdots O and N—H \cdots O hydrogen bonds (Table 1) form an extensive three-dimensional network, which consolidates the crystal packing.

Experimental

Disodium naphthalene-1,5-disulfonate (0.33 g, 1 mmol) and imidazole (0.27 g, 4 mmol) were added to an aqueous solution of $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.24 g, 1 mmol). The result solution was stirred at 60°C for four hours in a water bath. After filtration, a clear solution was set aside to crystallize. Platelike blue crystals were collected in 70% yield (base on Ni) after three days. Anal. Calcd for $\text{C}_{16}\text{H}_{22}\text{N}_4\text{O}_{10}\text{S}_2\text{Ni}$: C, 34.74; H, 4.01; N, 10.13; Found: C, 34.71; H, 4.06; N, 10.18.

Refinement

C- and N-bound H atoms were placed geometrically [C—H = 0.93 and N—H = 0.86 Å] and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N}, \text{C})$. Water H atoms were located on a difference map, and were refined isotropically with bond restraints O—H = 0.82 (2) Å and H \cdots H = 1.35 (2) Å.

Figures

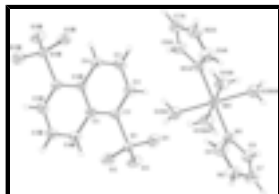


Fig. 1. View of the title compound with the atomic numbering and 30% probability displacement ellipsoids [symmetry codes: (A) $-x + 1, -y + 1, -z + 1$; (B) $-x + 1, -y, -z + 2$].

Tetraaquadimidazolenickel(II) naphthalene-1,5-disulfonate

Crystal data

$[\text{Ni}(\text{C}_3\text{H}_4\text{N}_2)_2(\text{H}_2\text{O})_4](\text{C}_{10}\text{H}_6\text{O}_6\text{S}_2)$	$Z = 1$
$M_r = 553.21$	$F_{000} = 286$
Triclinic, $P\bar{1}$	$D_x = 1.656 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.285 (3) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 8.925 (3) \text{ \AA}$	Cell parameters from 2499 reflections
$c = 9.088 (3) \text{ \AA}$	$\theta = 2.5\text{--}27.5^\circ$
$\alpha = 107.705 (5)^\circ$	$\mu = 1.12 \text{ mm}^{-1}$
$\beta = 101.628 (5)^\circ$	$T = 273 (2) \text{ K}$
$\gamma = 111.967 (5)^\circ$	Plate, blue
$V = 554.6 (3) \text{ \AA}^3$	$0.37 \times 0.28 \times 0.22 \text{ mm}$

Data collection

Bruker SMART 1K CCD diffractometer	2499 independent reflections
Radiation source: fine-focus sealed tube	2262 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.011$
$T = 273(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -10 \rightarrow 10$
$T_{\text{min}} = 0.681$, $T_{\text{max}} = 0.790$	$k = -11 \rightarrow 11$
4834 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.024$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0346P)^2 + 0.1772P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
2499 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
167 parameters	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
6 restraints	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	0.5000	0.5000	0.02611 (9)
N1	0.28615 (18)	0.55991 (17)	0.43827 (16)	0.0318 (3)
O1W	0.31627 (16)	0.23254 (16)	0.43179 (17)	0.0400 (3)
O2W	0.50259 (17)	0.42911 (17)	0.25854 (14)	0.0370 (3)
S1	0.21612 (5)	0.14229 (5)	0.81936 (4)	0.02708 (10)
C1	0.41626 (19)	0.11368 (19)	0.88348 (17)	0.0259 (3)
C5	0.41915 (19)	0.01134 (18)	0.97747 (17)	0.0248 (3)
O3	0.06491 (16)	-0.03557 (16)	0.71539 (15)	0.0406 (3)
O2	0.18864 (17)	0.22940 (17)	0.96754 (15)	0.0407 (3)
O1	0.25746 (18)	0.25029 (18)	0.72669 (17)	0.0436 (3)
N2	0.1179 (2)	0.6991 (2)	0.4648 (2)	0.0478 (4)
H7A	0.0826	0.7757	0.5081	0.057*
C2	0.5648 (2)	0.1890 (2)	0.8392 (2)	0.0353 (3)
H2A	0.5610	0.2560	0.7789	0.042*
C3	0.7231 (2)	0.1653 (2)	0.8846 (2)	0.0390 (4)
H3A	0.8235	0.2169	0.8541	0.047*
C7	0.0278 (3)	0.5634 (3)	0.3116 (3)	0.0449 (4)
H2B	-0.0831	0.5350	0.2335	0.054*
C8	0.1323 (2)	0.4782 (2)	0.2957 (2)	0.0384 (4)
H8A	0.1045	0.3792	0.2025	0.046*
C6	0.2709 (3)	0.6926 (3)	0.5365 (2)	0.0459 (4)
H6A	0.3560	0.7719	0.6425	0.055*
C4	0.7313 (2)	0.0678 (2)	0.9726 (2)	0.0317 (3)
H4A	0.8366	0.0526	1.0006	0.038*
H2WA	0.570 (3)	0.510 (2)	0.241 (3)	0.057 (7)*
H2WB	0.402 (3)	0.368 (3)	0.176 (3)	0.054 (6)*
H1WA	0.215 (2)	0.179 (3)	0.357 (2)	0.062 (7)*
H1WB	0.302 (3)	0.211 (4)	0.511 (2)	0.075 (9)*

Atomic displacement parameters (\AA^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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supplementary materials

Ni1	0.02173 (14)	0.02598 (14)	0.02342 (14)	0.00944 (11)	0.00564 (10)	0.00513 (10)
N1	0.0287 (6)	0.0320 (7)	0.0311 (6)	0.0147 (5)	0.0101 (5)	0.0084 (5)
O1W	0.0273 (6)	0.0327 (6)	0.0433 (7)	0.0060 (5)	0.0060 (5)	0.0096 (5)
O2W	0.0350 (6)	0.0404 (7)	0.0274 (6)	0.0143 (5)	0.0094 (5)	0.0094 (5)
S1	0.02158 (17)	0.02921 (19)	0.02718 (19)	0.01217 (14)	0.00530 (14)	0.00956 (14)
C1	0.0207 (6)	0.0278 (7)	0.0256 (7)	0.0112 (5)	0.0059 (5)	0.0086 (5)
C5	0.0207 (6)	0.0249 (7)	0.0235 (6)	0.0089 (5)	0.0068 (5)	0.0063 (5)
O3	0.0256 (5)	0.0360 (6)	0.0415 (7)	0.0106 (5)	0.0003 (5)	0.0055 (5)
O2	0.0353 (6)	0.0498 (7)	0.0359 (6)	0.0267 (6)	0.0115 (5)	0.0088 (5)
O1	0.0405 (7)	0.0530 (7)	0.0522 (7)	0.0265 (6)	0.0175 (6)	0.0337 (6)
N2	0.0513 (9)	0.0465 (9)	0.0621 (10)	0.0348 (8)	0.0301 (8)	0.0216 (8)
C2	0.0299 (8)	0.0428 (9)	0.0413 (9)	0.0175 (7)	0.0154 (7)	0.0251 (7)
C3	0.0267 (8)	0.0513 (10)	0.0506 (10)	0.0182 (7)	0.0214 (7)	0.0308 (8)
C7	0.0343 (9)	0.0536 (11)	0.0540 (11)	0.0253 (8)	0.0156 (8)	0.0254 (9)
C8	0.0304 (8)	0.0403 (9)	0.0368 (9)	0.0181 (7)	0.0064 (7)	0.0083 (7)
C6	0.0470 (10)	0.0432 (10)	0.0400 (9)	0.0251 (8)	0.0129 (8)	0.0049 (8)
C4	0.0215 (7)	0.0382 (8)	0.0372 (8)	0.0145 (6)	0.0116 (6)	0.0168 (7)

Geometric parameters (Å, °)

Ni1—Ni ⁱ	2.0568 (14)	C1—C5	1.431 (2)
Ni1—N1	2.0568 (14)	C5—C4 ⁱⁱ	1.422 (2)
Ni1—O2W ⁱ	2.0979 (13)	C5—C5 ⁱⁱ	1.427 (3)
Ni1—O2W	2.0979 (13)	N2—C6	1.334 (2)
Ni1—O1W	2.0978 (13)	N2—C7	1.357 (3)
Ni1—O1W ⁱ	2.0978 (13)	N2—H7A	0.8600
N1—C6	1.315 (2)	C2—C3	1.407 (2)
N1—C8	1.378 (2)	C2—H2A	0.9300
O1W—H1WA	0.82 (2)	C3—C4	1.359 (2)
O1W—H1WB	0.82 (2)	C3—H3A	0.9300
O2W—H2WA	0.81 (2)	C7—C8	1.351 (2)
O2W—H2WB	0.81 (2)	C7—H2B	0.9300
S1—O2	1.4453 (12)	C8—H8A	0.9300
S1—O3	1.4508 (13)	C6—H6A	0.9300
S1—O1	1.4556 (13)	C4—C5 ⁱⁱ	1.422 (2)
S1—C1	1.7811 (15)	C4—H4A	0.9300
C1—C2	1.369 (2)		
N1 ⁱ —Ni1—N1	180.0	O1—S1—C1	106.33 (7)
N1 ⁱ —Ni1—O2W ⁱ	91.34 (5)	C2—C1—C5	121.07 (13)
N1—Ni1—O2W ⁱ	88.66 (5)	C2—C1—S1	118.79 (12)
N1 ⁱ —Ni1—O2W	88.66 (5)	C5—C1—S1	120.14 (10)
N1—Ni1—O2W	91.34 (5)	C4 ⁱⁱ —C5—C5 ⁱⁱ	119.05 (17)
O2W ⁱ —Ni1—O2W	180.0	C4 ⁱⁱ —C5—C1	122.89 (13)
N1 ⁱ —Ni1—O1W	87.22 (6)	C5 ⁱⁱ —C5—C1	118.05 (16)
N1—Ni1—O1W	92.78 (6)	C6—N2—C7	107.87 (15)
O2W ⁱ —Ni1—O1W	91.48 (5)	C6—N2—H7A	126.1

O2W—Ni1—O1W	88.52 (5)	C7—N2—H7A	126.1
N1 ⁱ —Ni1—O1W ⁱ	92.78 (6)	C1—C2—C3	120.14 (15)
N1—Ni1—O1W ⁱ	87.22 (6)	C1—C2—H2A	119.9
O2W ⁱ —Ni1—O1W ⁱ	88.52 (5)	C3—C2—H2A	119.9
O2W—Ni1—O1W ⁱ	91.48 (5)	C4—C3—C2	120.80 (14)
O1W—Ni1—O1W ⁱ	180.0	C4—C3—H3A	119.6
C6—N1—C8	104.96 (14)	C2—C3—H3A	119.6
C6—N1—Ni1	124.39 (12)	C8—C7—N2	105.88 (16)
C8—N1—Ni1	130.65 (11)	C8—C7—H2B	127.1
Ni1—O1W—H1WA	122.5 (16)	N2—C7—H2B	127.1
Ni1—O1W—H1WB	113.1 (19)	C7—C8—N1	109.81 (16)
H1WA—O1W—H1WB	107.7 (19)	C7—C8—H8A	125.1
Ni1—O2W—H2WA	115.4 (16)	N1—C8—H8A	125.1
Ni1—O2W—H2WB	121.1 (15)	N1—C6—N2	111.48 (16)
H2WA—O2W—H2WB	106.8 (18)	N1—C6—H6A	124.3
O2—S1—O3	113.08 (8)	N2—C6—H6A	124.3
O2—S1—O1	112.57 (8)	C3—C4—C5 ⁱⁱ	120.88 (14)
O3—S1—O1	111.83 (8)	C3—C4—H4A	119.6
O2—S1—C1	106.98 (7)	C5 ⁱⁱ —C4—H4A	119.6
O3—S1—C1	105.41 (7)		
O2W ⁱ —Ni1—N1—C6	37.27 (15)	S1—C1—C5—C4 ⁱⁱ	-1.5 (2)
O2W—Ni1—N1—C6	-142.73 (15)	C2—C1—C5—C5 ⁱⁱ	-0.5 (2)
O1W—Ni1—N1—C6	128.69 (15)	S1—C1—C5—C5 ⁱⁱ	178.52 (13)
O1W ⁱ —Ni1—N1—C6	-51.31 (15)	C5—C1—C2—C3	0.6 (2)
O2W ⁱ —Ni1—N1—C8	-142.13 (15)	S1—C1—C2—C3	-178.51 (14)
O2W—Ni1—N1—C8	37.87 (15)	C1—C2—C3—C4	0.0 (3)
O1W—Ni1—N1—C8	-50.71 (15)	C6—N2—C7—C8	-0.1 (2)
O1W ⁱ —Ni1—N1—C8	129.29 (15)	N2—C7—C8—N1	0.2 (2)
O2—S1—C1—C2	-121.03 (14)	C6—N1—C8—C7	-0.1 (2)
O3—S1—C1—C2	118.35 (14)	Ni1—N1—C8—C7	179.38 (12)
O1—S1—C1—C2	-0.52 (15)	C8—N1—C6—N2	0.0 (2)
O2—S1—C1—C5	59.89 (13)	Ni1—N1—C6—N2	-179.51 (12)
O3—S1—C1—C5	-60.73 (13)	C7—N2—C6—N1	0.1 (2)
O1—S1—C1—C5	-179.60 (12)	C2—C3—C4—C5 ⁱⁱ	-0.6 (3)
C2—C1—C5—C4 ⁱⁱ	179.40 (15)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1W—H1WA \cdots O3 ⁱⁱⁱ	0.82 (2)	2.022 (15)	2.7507 (18)	148 (2)
O1W—H1WB \cdots O1	0.82 (2)	2.018 (14)	2.788 (2)	156 (3)
O2W—H2WA \cdots O1 ⁱ	0.81 (2)	1.962 (10)	2.7496 (19)	161 (2)
O2W—H2WB \cdots O2 ^{iv}	0.81 (2)	1.96 (2)	2.7979 (18)	173 (2)
N2—H7A \cdots O3 ^v	0.86	2.19	2.981 (2)	154

supplementary materials

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

Fig. 1

