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Bis(4-aminobenzenesulfonato-κN)tetraaquanickel(II)

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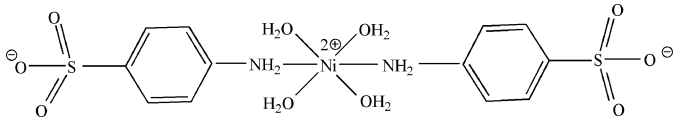
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.030; wR factor = 0.091; data-to-parameter ratio = 14.3.

In the title complex, $[Ni(C_6H_2O_3S)_2(H_2O)_4]$, the Ni^{II} atom is octahedrally coordinated by two 4-aminobenzenesulfonate N atoms and four water molecules. The molecular complex is centrosymmetic, with the Ni^{II} ion located on an inversion centre.

Related literature

For related literature, see: Gunderman *et al.* (1996); Shakeri & Haussuhl (1992*a*, 1992*b*); Zhou *et al.* (2004).



Experimental

Crystal data

$[Ni(C_6H_2O_3S)_2(H_2O)_4]$
M_r = 475.13
Monoclinic, $C2/c$
a = 20.800 (11) Å
b = 6.450 (3) Å
c = 13.566 (7) Å
β = 106.593 (9)°
V = 1744.1 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 293 (2) K
0.18 × 0.12 × 0.08 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.735, T_{max} = 1.000
(expected range = 0.656–0.893)
6482 measured reflections
1997 independent reflections
1722 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.091
S = 1.00
1997 reflections
140 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O5	2.060 (2)	Ni1—N1	2.133 (3)
Ni1—O4	2.064 (2)		
O5—Ni1—O4	89.45 (9)	O4—Ni1—N1	90.66 (10)
O5—Ni1—N1	84.45 (9)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{ii}	0.900 (10)	2.215 (15)	3.084 (4)	162 (3)
N1—H1B···O3^{iii}	0.905 (10)	2.209 (13)	3.106 (4)	171 (4)
O4—H4A···S1^{iii}	0.84	2.96	3.768 (3)	161
O4—H4B···O1^{iv}	0.898 (10)	1.896 (14)	2.777 (3)	166 (2)
O4—H4B···S1^{iv}	0.898 (10)	2.82 (3)	3.595 (3)	145 (3)
O5—H5A···O3^{iv}	0.84	1.94	2.773 (3)	169
O5—H5B···O1^{v}	0.908 (10)	1.927 (11)	2.834 (3)	177 (4)

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1999); 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: BV2057).

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supplementary materials

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Bis(4-aminobenzenesulfonato-κN)tetraaquanickel(II)

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Comment

The 4-aminobenzenesulfonic acid can bind to transition metals through the amino as well as the carboxylate ends. Crystal structures of metal and 4-aminobenzenesulfonic acid that have been reported include, for example, $(C_{12}H_{16}CdN_2O_8S_2)_n$ (Zhou, *et al.*,2004), $[Cu(H_2NC_6H_4SO_3)_2(H_2O)_2]\cdot 2H_2O$ and $[Mn(H_2NC_6H_4SO_3)_2(H_2O)_2]$ (Gunderman *et al.*, 1996). In two other derivatives, the isostructural compounds $[M(H_2NC_6H_4SO_3)_2(H_2O)_2]\cdot 2H_2O$ (*M*=Co, Zn; Shakeri & Haussuhl, 1992*a*; Shakeri & Haussuhl, 1992*b*), both ends engage in coordination.

The reaction of the sulfanilic anion with nickel(II) gives the title compound, in which the anion coordinates through the amine group. There are extensive hydrogen bonds (N—H···O, O—H···O) in the title compound. The sulfonic O atoms are linked to the coordinated water molecules and 4-aminobenzenesulfonic acid N atoms by H bonds. The complex attains a three-dimensional supramolecular by hydrogen bonds (Fig.2).

Experimental

A mixture of nickel(II) chloride hexahydrate (0.24 g, 1 mmol), sodium hydroxide (0.08 g, 2 mmol), sulfanilic acid (0.17 g, 1 mmol) and water (17 mmol) was placed in a Teflon-lined stainless-steel bomb. The bomb was heated at 343 K for 72 h. Red crystals suitable for single-crystal X-ray analysis were isolated from the cool solution in about 50% yield.

Refinement

H atoms attached to C atoms were placed in calculated positions and treated using a riding-model approximation (C—H = 0.95 for benzene ring H atoms with U_{iso}(H) = 1.2Ueq(C)). The H atoms bonded to O atoms were visible in the difference Fourier map and were included in the refinement with O—H distance restraint of 0.90, and with U_{iso}(H) = 1.5Ueq(O). The amine protons were refined isotropically.

Figures

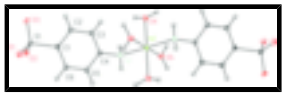

Fig. 1. *ORTEP* diagram of the title compound with atoms drawn as 30% probability ellipsoids (H atoms are not labled).

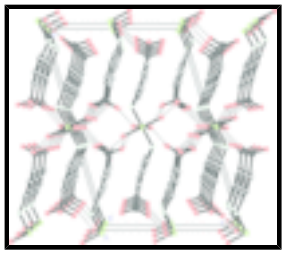

Fig. 2. The three-dimensional net work structure formed by the hydrogen bonds(all H atoms were omitted for clarity).

Bis(4-aminobenzenesulfonato-κ*N*)tetraaquanickel(II)

Crystal data

$[Ni(C_6H_2O_3S)_2(H_2O)_4]$	F_{000} = 984
M_r = 475.13	D_x = 1.809 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 20.800 (11) Å	Cell parameters from 2071 reflections
b = 6.450 (3) Å	θ = 2.0–27.5º
c = 13.566 (7) Å	μ = 1.41 mm^{-1}
β = 106.593 (9)º	*T* = 293 (2) K
V = 1744.1 (15) Å^3	Prism, green
Z = 4	0.18 × 0.12 × 0.08 mm

Data collection

Bruker SMART diffractometer	1997 independent reflections
Radiation source: fine-focus sealed tube	1722 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 14.6306 pixels mm^{-1}	θ_{max} = 27.5º
T = 173(2) K	θ_{min} = 2.0º
CCD_Profile_fitting scans	*h* = −26→26
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*k* = −7→8
T_{min} = 0.735, T_{max} = 1.000	*l* = −17→17
6482 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
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.091	$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 10.4033P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.030
1997 reflections	$\Delta\rho_{max}$ = 0.44 e Å^{-3}
140 parameters	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
9 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.5000	0.0000	1.0000	0.01645 (14)
S1	0.87523 (3)	−0.09331 (11)	1.20823 (6)	0.01997 (17)
N1	0.59233 (12)	0.0734 (4)	0.96894 (19)	0.0206 (5)
H1A	0.5919 (18)	0.2081 (18)	0.951 (2)	0.029 (9)*
H1B	0.596 (2)	−0.010 (4)	0.917 (2)	0.057 (14)*
C1	0.78851 (14)	−0.0450 (5)	1.1547 (2)	0.0192 (6)
C2	0.74470 (15)	−0.2073 (5)	1.1195 (3)	0.0278 (7)
H2A	0.7593	−0.3463	1.1345	0.033*
C3	0.67935 (15)	−0.1665 (5)	1.0622 (2)	0.0257 (7)
H3A	0.6490	−0.2780	1.0386	0.031*
C4	0.65795 (13)	0.0354 (4)	1.0390 (2)	0.0186 (6)
C5	0.70049 (15)	0.1979 (5)	1.0810 (2)	0.0258 (6)
H5C	0.6848	0.3367	1.0703	0.031*
C6	0.76580 (15)	0.1582 (5)	1.1385 (2)	0.0256 (7)
H6A	0.7951	0.2697	1.1669	0.031*
O1	0.89542 (11)	0.0018 (4)	1.31048 (17)	0.0283 (5)
O2	0.90761 (11)	0.0044 (4)	1.13772 (19)	0.0306 (5)
O3	0.88359 (11)	−0.3179 (3)	1.21135 (17)	0.0277 (5)
O4	0.50276 (11)	−0.2964 (3)	0.94394 (17)	0.0264 (5)
H4A	0.5372	−0.3104	0.9241	0.040*
H4B	0.4639 (7)	−0.353 (7)	0.907 (3)	0.064 (15)*
O5	0.45678 (11)	0.1030 (3)	0.85214 (16)	0.0251 (5)
H5A	0.4360	0.0050	0.8160	0.038*
H5B	0.4369 (15)	0.2296 (19)	0.841 (3)	0.058 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0141 (2)	0.0153 (2)	0.0175 (3)	0.0006 (2)	0.00051 (18)	−0.0002 (2)
S1	0.0164 (3)	0.0181 (3)	0.0224 (4)	0.0030 (3)	0.0008 (3)	0.0010 (3)
N1	0.0171 (11)	0.0202 (12)	0.0223 (12)	0.0002 (10)	0.0021 (10)	0.0019 (10)
C1	0.0148 (12)	0.0233 (15)	0.0171 (13)	0.0014 (11)	0.0008 (10)	−0.0003 (11)

C2	0.0247 (15)	0.0174 (14)	0.0364 (18)	0.0034 (12)	0.0011 (13)	0.0044 (13)
C3	0.0202 (14)	0.0199 (14)	0.0330 (17)	−0.0040 (12)	0.0011 (12)	−0.0011 (13)
C4	0.0145 (12)	0.0223 (15)	0.0191 (13)	0.0021 (11)	0.0049 (10)	0.0010 (11)
C5	0.0222 (14)	0.0191 (14)	0.0332 (17)	0.0048 (12)	0.0033 (12)	−0.0016 (13)
C6	0.0203 (14)	0.0199 (14)	0.0324 (17)	−0.0018 (12)	0.0009 (12)	−0.0050 (13)
O1	0.0256 (11)	0.0279 (12)	0.0257 (11)	0.0014 (10)	−0.0018 (9)	−0.0051 (10)
O2	0.0240 (11)	0.0306 (12)	0.0392 (13)	0.0041 (10)	0.0125 (10)	0.0084 (11)
O3	0.0289 (11)	0.0194 (11)	0.0292 (12)	0.0073 (9)	−0.0005 (9)	0.0005 (9)
O4	0.0239 (10)	0.0200 (11)	0.0341 (12)	−0.0023 (9)	0.0065 (9)	−0.0085 (9)
O5	0.0285 (11)	0.0200 (11)	0.0209 (11)	0.0016 (9)	−0.0025 (9)	0.0004 (9)

Geometric parameters (Å, °)

Ni1—O5	2.060 (2)	C1—C6	1.389 (4)
Ni1—O5^{i}	2.060 (2)	C2—C3	1.385 (4)
Ni1—O4	2.064 (2)	C2—H2A	0.9500
Ni1—O4^{i}	2.064 (2)	C3—C4	1.384 (4)
Ni1—N1^{i}	2.133 (3)	C3—H3A	0.9500
Ni1—N1	2.133 (3)	C4—C5	1.385 (4)
S1—O3	1.458 (2)	C5—C6	1.384 (4)
S1—O2	1.461 (2)	C5—H5C	0.9500
S1—O1	1.464 (2)	C6—H6A	0.9500
S1—C1	1.769 (3)	O4—H4A	0.8400
N1—C4	1.444 (4)	O4—H4B	0.898 (10)
N1—H1A	0.900 (10)	O5—H5A	0.8400
N1—H1B	0.905 (10)	O5—H5B	0.908 (10)
C1—C2	1.381 (4)		
O5—Ni1—O5^{i}	180.000 (1)	H1A—N1—H1B	111.5 (16)
O5—Ni1—O4	89.45 (9)	C2—C1—C6	120.0 (3)
O5^{i}—Ni1—O4	90.55 (9)	C2—C1—S1	120.2 (2)
O5—Ni1—O4^{i}	90.55 (9)	C6—C1—S1	119.5 (2)
O5^{i}—Ni1—O4^{i}	89.45 (9)	C1—C2—C3	119.7 (3)
O4—Ni1—O4^{i}	180.0	C1—C2—H2A	120.1
O5—Ni1—N1^{i}	95.55 (9)	C3—C2—H2A	120.1
O5^{i}—Ni1—N1^{i}	84.45 (9)	C4—C3—C2	120.5 (3)
O4—Ni1—N1^{i}	89.34 (10)	C4—C3—H3A	119.8
O4^{i}—Ni1—N1^{i}	90.66 (10)	C2—C3—H3A	119.8
O5—Ni1—N1	84.45 (9)	C3—C4—C5	119.5 (3)
O5^{i}—Ni1—N1	95.55 (9)	C3—C4—N1	119.4 (3)
O4—Ni1—N1	90.66 (10)	C5—C4—N1	121.0 (3)
O4^{i}—Ni1—N1	89.34 (10)	C6—C5—C4	120.1 (3)
N1^{i}—Ni1—N1	180.000 (1)	C6—C5—H5C	120.0
O3—S1—O2	111.96 (14)	C4—C5—H5C	120.0
O3—S1—O1	112.91 (14)	C5—C6—C1	119.9 (3)
O2—S1—O1	112.23 (15)	C5—C6—H6A	120.0
O3—S1—C1	106.63 (14)	C1—C6—H6A	120.0

O2—S1—C1	105.20 (14)	Ni1—O4—H4A	109.5
O1—S1—C1	107.33 (13)	Ni1—O4—H4B	118 (2)
C4—N1—Ni1	124.58 (19)	H4A—O4—H4B	119.4
C4—N1—H1A	106 (2)	Ni1—O5—H5A	109.5
Ni1—N1—H1A	109 (2)	Ni1—O5—H5B	120 (2)
C4—N1—H1B	98 (3)	H5A—O5—H5B	116.5
Ni1—N1—H1B	107 (3)		
O5—Ni1—N1—C4	−176.5 (2)	S1—C1—C2—C3	−169.0 (3)
O5^{i}—Ni1—N1—C4	3.5 (2)	C1—C2—C3—C4	0.8 (5)
O4—Ni1—N1—C4	−87.1 (2)	C2—C3—C4—C5	−5.7 (5)
O4^{i}—Ni1—N1—C4	92.9 (2)	C2—C3—C4—N1	172.5 (3)
N1^{i}—Ni1—N1—C4	11 (100)	Ni1—N1—C4—C3	66.7 (4)
O3—S1—C1—C2	−4.2 (3)	Ni1—N1—C4—C5	−115.1 (3)
O2—S1—C1—C2	114.9 (3)	C3—C4—C5—C6	5.5 (5)
O1—S1—C1—C2	−125.4 (3)	N1—C4—C5—C6	−172.7 (3)
O3—S1—C1—C6	−177.5 (2)	C4—C5—C6—C1	−0.4 (5)
O2—S1—C1—C6	−58.4 (3)	C2—C1—C6—C5	−4.5 (5)
O1—S1—C1—C6	61.3 (3)	S1—C1—C6—C5	168.8 (2)
C6—C1—C2—C3	4.3 (5)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{ii}	0.900 (10)	2.215 (15)	3.084 (4)	162 (3)
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O4—H4B···S1^{iv}	0.898 (10)	2.82 (3)	3.595 (3)	145 (3)
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O5—H5B···O1^{v}	0.908 (10)	1.927 (11)	2.834 (3)	177 (4)

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

Fig. 1

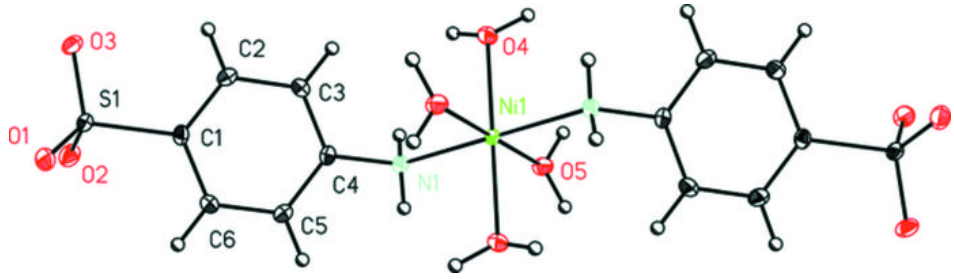

Fig. 2