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Bis[2-(2-pyridylmethylamino)ethanesulfonato-κ^3N,N',O]nickel(II)

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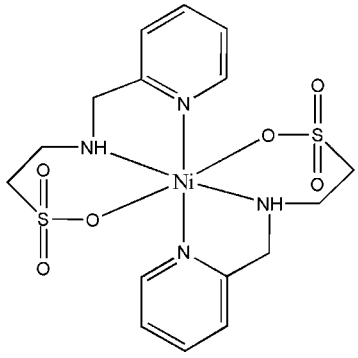
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.068; data-to-parameter ratio = 17.5.

In mononuclear $[Ni(C_8H_{11}N_2O_3S)_2]$, a nickel(II) complex of 2-(2-pyridylmethylamino)ethanesulfonic acid, the six-coordinate Ni atom lies on a centre of symmetry. The monodeprotonated anion coordinates in a *facial* arrangement through two N and one O atoms. Intermolecular N—H···O hydrogen bonds are present in the crystal structure.

Related literature

For the isostuctural cobalt(II) analogue, see: Li *et al.* (2006).



Experimental

Crystal data

$[Ni(C_8H_{11}N_2O_3S)_2]$
M_r = 489.21
Monoclinic, $P2_1/c$
a = 9.6090 (10) Å
b = 9.9270 (10) Å
c = 11.4537 (12) Å
β = 106.8480 (10)°
V = 1045.66 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.17 mm^{-1}
T = 291 (2) K
0.35 × 0.26 × 0.22 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.683, T_{max} = 0.787
8966 measured reflections
2401 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.068
S = 1.04
2401 reflections
137 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O3	2.0879 (11)	Ni1—N1	2.1253 (13)
Ni1—N2	2.1116 (12)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1N···O1^{i}	0.847 (18)	2.100 (19)	2.9394 (17)	170.6 (16)

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); 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: NG2282).

References

Bruker (2004). *APEX2* (Version 2004/1), *SAINT* (Version 7.12a) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
Li, J.-X., Jiang, Y.-M. & Li, H.-Y. (2006). *Acta Cryst.* E**62**, m2984–m2986.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807029911

supplementary materials

Acta Cryst. (2007). E**63**, m1974 [**doi:10.1107/S1600536807029911**]

Bis[2-(2-pyridylmethylamino)ethanesulfonato-κ^3N,N',O]nickel(II)

B.-L. Liao, J.-X. Li and Y.-M. Jiang

Comment

The compound is isostructural with $[Co(C_8H_{11}N_2O_3S)_2]$, whose structure has been described in detail (Li *et al.*, 2006)·The six-coordiante nickel atom lies on an inversion centre with the two monodeprotonated lingds coordinate in a tridentate facial arrangement with its three donor atoms.

The N—H donor and S═O acceptor groups of the PMT ligand participate in the hydrogen bonding and form a two-dimensional network in the *bc* plane (Fig. 2 and Table 2).

Experimental

2-(2-Pyridylmethylamino)ethanesulfonic acid was prepared according to the method of Li *et al.,* 2006). The ligand (2.0 mmol, 0.432 g) was dissolved in water (15 ml). To this solution, $NiCl_26H_2O$ (1.0 m mol, 0.238 g) was added, and the resulting mixture was stirred at 323 K for 6 h. The solution was filtered; the filtrate was left to stand at room temperature. Green block-shaped crystals were obtained in a yield of 43%. Analysis, found(%): C 39.31; H 4.54; N 11.38; S 13.01. $C_{16}H_{22}NiN_4O_6S_2$ requires(%): C 39.25; H 4.50; N 11.45; S 13.08. IR(KBr, ν cm^{-1}):771.3[γ(C═C—H)], 746.5(γ CH_2); 1189.5, 1149.5, 1035.1(ν SO_3^-); 1608.7, 1571.8 (ν C═ C+C═N); 3213.8 (νN-H).

Refinement

H atoms bonded to C were positioned geometrically with C—H distance 0.93–0.97 Å, and treated as riding atoms, with $U_{iso}(H)=1.2U_{eq}(C)$. The N—H hydrogen atom was located in a difference Fourier map and refined isotropically.

Figures

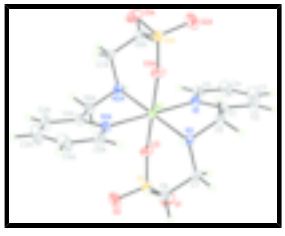

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Symmetry code:(i)-*x*, −*y*, −*z*.

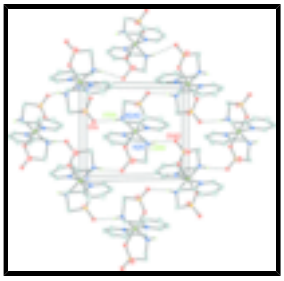

Fig. 2. Packing of (I), showing the two-dimensional sheet structure in the *bc* plane, linked *via* hydrogen bonds (dashed lines). H atoms bonded to C atoms have been omitted.

Bis[2-(2-pyridylmethylamino)ethanesulfonato- κ^3N,N',O]nickel(II)

Crystal data

$[Ni(C_8H_{11}N_2O_3S)_2]$	F_{000} = 508
M_r = 489.21	D_x = 1.554 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5566 reflections
a = 9.6090 (10) Å	θ = 2.8–28.2º
b = 9.9270 (10) Å	μ = 1.17 mm^{-1}
c = 11.4537 (12) Å	T = 291 (2) K
β = 106.8480 (10)º	Block, green
V = 1045.66 (19) Å^3	0.35 × 0.26 × 0.22 mm
Z = 2	

Data collection

Bruker APEX II CCD area-detector diffractometer	2401 independent reflections
Radiation source: fine-focus sealed tube	2212 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.016
T = 291(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.683, T_{max} = 0.787	k = −12→12
8966 measured reflections	l = −14→14

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
$wR(F^2)$ = 0.068	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.3431P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$

2401 reflections	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
137 parameters	$\Delta\rho_{min}$ = −0.38 e Å^{-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 $F^2 > \sigma(F^2)$ 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	0.0000	0.0000	0.0000	0.02225 (9)
S1	−0.13109 (4)	0.28994 (4)	0.04303 (3)	0.02938 (10)
O1	−0.05360 (16)	0.39933 (12)	0.11905 (10)	0.0458 (3)
O2	−0.28622 (14)	0.29309 (16)	0.02363 (14)	0.0588 (4)
O3	−0.06507 (13)	0.15954 (11)	0.09085 (10)	0.0356 (2)
N1	0.21837 (14)	0.03407 (13)	0.10617 (12)	0.0303 (3)
N2	0.07293 (13)	0.13004 (12)	−0.11590 (11)	0.0278 (2)
C1	0.30118 (16)	0.08851 (16)	0.04133 (16)	0.0361 (3)
C2	0.4419 (2)	0.1324 (2)	0.0964 (2)	0.0603 (6)
H2	0.4970	0.1706	0.0503	0.072*
C3	0.4988 (2)	0.1182 (3)	0.2214 (2)	0.0772 (8)
H3	0.5929	0.1473	0.2603	0.093*
C4	0.4153 (2)	0.0608 (3)	0.2882 (2)	0.0639 (6)
H4	0.4525	0.0498	0.3721	0.077*
C5	0.2757 (2)	0.01988 (18)	0.22770 (16)	0.0405 (4)

H5	0.2192	−0.0188	0.2724	0.049*
C6	0.22948 (17)	0.09836 (17)	−0.09381 (15)	0.0371 (3)
H6A	0.2757	0.1685	−0.1284	0.045*
H6B	0.2399	0.0137	−0.1328	0.045*
C7	0.05421 (17)	0.27742 (14)	−0.10031 (14)	0.0316 (3)
H7A	0.0786	0.3259	−0.1653	0.038*
H7B	0.1206	0.3065	−0.0234	0.038*
C8	−0.10033 (17)	0.31163 (15)	−0.10230 (13)	0.0303 (3)
H8A	−0.1672	0.2546	−0.1615	0.036*
H8B	−0.1207	0.4044	−0.1282	0.036*
H1N	0.0333 (19)	0.1125 (17)	−0.1905 (17)	0.033 (4)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.02352 (14)	0.02147 (14)	0.02214 (13)	−0.00247 (8)	0.00720 (10)	0.00056 (8)
S1	0.0344 (2)	0.02661 (18)	0.02887 (18)	0.00052 (13)	0.01194 (14)	−0.00103 (13)
O1	0.0754 (9)	0.0310 (6)	0.0330 (6)	−0.0097 (6)	0.0188 (6)	−0.0074 (5)
O2	0.0368 (7)	0.0803 (11)	0.0640 (9)	0.0074 (7)	0.0221 (6)	0.0116 (8)
O3	0.0550 (7)	0.0273 (5)	0.0282 (5)	0.0044 (5)	0.0179 (5)	0.0016 (4)
N1	0.0269 (6)	0.0304 (6)	0.0321 (6)	−0.0018 (5)	0.0064 (5)	−0.0012 (5)
N2	0.0321 (6)	0.0272 (6)	0.0253 (6)	−0.0023 (5)	0.0103 (5)	0.0003 (5)
C1	0.0268 (7)	0.0356 (8)	0.0475 (9)	−0.0008 (6)	0.0129 (6)	−0.0004 (7)
C2	0.0296 (9)	0.0726 (14)	0.0790 (15)	−0.0126 (9)	0.0163 (9)	−0.0016 (12)
C3	0.0305 (10)	0.107 (2)	0.0793 (17)	−0.0160 (11)	−0.0067 (10)	−0.0112 (15)
C4	0.0437 (11)	0.0867 (16)	0.0464 (11)	0.0005 (11)	−0.0106 (9)	−0.0070 (11)
C5	0.0378 (9)	0.0444 (9)	0.0350 (8)	0.0026 (7)	0.0037 (7)	−0.0020 (7)
C6	0.0350 (8)	0.0394 (8)	0.0444 (9)	−0.0021 (6)	0.0232 (7)	0.0029 (7)
C7	0.0393 (8)	0.0251 (7)	0.0326 (7)	−0.0047 (6)	0.0140 (6)	0.0025 (6)
C8	0.0373 (8)	0.0274 (7)	0.0247 (6)	0.0020 (6)	0.0065 (6)	0.0028 (5)

Geometric parameters (Å, °)

Ni1—O3	2.0879 (11)	C1—C6	1.504 (2)
Ni1—O3^{i}	2.0879 (11)	C2—C3	1.383 (3)
Ni1—N2	2.1116 (12)	C2—H2	0.9300
Ni1—N2^{i}	2.1117 (12)	C3—C4	1.382 (4)
Ni1—N1^{i}	2.1253 (13)	C3—H3	0.9300
Ni1—N1	2.1253 (13)	C4—C5	1.380 (3)
S1—O2	1.4424 (13)	C4—H4	0.9300
S1—O1	1.4547 (12)	C5—H5	0.9300
S1—O3	1.4753 (11)	C6—H6A	0.9700
S1—C8	1.7860 (15)	C6—H6B	0.9700
N1—C5	1.348 (2)	C7—C8	1.517 (2)
N1—C1	1.349 (2)	C7—H7A	0.9700
N2—C6	1.4849 (19)	C7—H7B	0.9700
N2—C7	1.4911 (19)	C8—H8A	0.9700
N2—H1N	0.847 (18)	C8—H8B	0.9700

C1—C2	1.387 (2)		
O3—Ni1—O3^{i}	180.0	N1—C1—C6	115.17 (13)
O3—Ni1—N2	92.95 (4)	C2—C1—C6	122.92 (16)
O3^{i}—Ni1—N2	87.05 (4)	C3—C2—C1	118.7 (2)
O3—Ni1—N2^{i}	87.05 (4)	C3—C2—H2	120.7
O3^{i}—Ni1—N2^{i}	92.95 (4)	C1—C2—H2	120.7
N2—Ni1—N2^{i}	180.00 (6)	C4—C3—C2	119.74 (19)
O3—Ni1—N1^{i}	90.99 (5)	C4—C3—H3	120.1
O3^{i}—Ni1—N1^{i}	89.01 (5)	C2—C3—H3	120.1
N2—Ni1—N1^{i}	100.96 (5)	C5—C4—C3	118.6 (2)
N2^{i}—Ni1—N1^{i}	79.04 (5)	C5—C4—H4	120.7
O3—Ni1—N1	89.01 (5)	C3—C4—H4	120.7
O3^{i}—Ni1—N1	90.99 (5)	N1—C5—C4	122.30 (19)
N2—Ni1—N1	79.04 (5)	N1—C5—H5	118.9
N2^{i}—Ni1—N1	100.96 (5)	C4—C5—H5	118.9
N1^{i}—Ni1—N1	180.0	N2—C6—C1	109.17 (12)
O2—S1—O1	113.76 (9)	N2—C6—H6A	109.8
O2—S1—O3	112.97 (8)	C1—C6—H6A	109.8
O1—S1—O3	110.02 (7)	N2—C6—H6B	109.8
O2—S1—C8	107.25 (8)	C1—C6—H6B	109.8
O1—S1—C8	105.88 (7)	H6A—C6—H6B	108.3
O3—S1—C8	106.40 (7)	N2—C7—C8	111.68 (12)
S1—O3—Ni1	129.73 (6)	N2—C7—H7A	109.3
C5—N1—C1	118.73 (14)	C8—C7—H7A	109.3
C5—N1—Ni1	127.92 (11)	N2—C7—H7B	109.3
C1—N1—Ni1	113.01 (10)	C8—C7—H7B	109.3
C6—N2—C7	109.81 (12)	H7A—C7—H7B	107.9
C6—N2—Ni1	105.53 (9)	C7—C8—S1	112.62 (10)
C7—N2—Ni1	116.81 (9)	C7—C8—H8A	109.1
C6—N2—H1N	105.4 (12)	S1—C8—H8A	109.1
C7—N2—H1N	106.7 (12)	C7—C8—H8B	109.1
Ni1—N2—H1N	112.0 (12)	S1—C8—H8B	109.1
N1—C1—C2	121.91 (17)	H8A—C8—H8B	107.8
O2—S1—O3—Ni1	101.05 (11)	N2^{i}—Ni1—N2—C7	160 (17)
O1—S1—O3—Ni1	−130.63 (9)	N1^{i}—Ni1—N2—C7	90.36 (11)
C8—S1—O3—Ni1	−16.37 (11)	N1—Ni1—N2—C7	−89.64 (11)
O3^{i}—Ni1—O3—S1	−153 (8)	C5—N1—C1—C2	−1.3 (3)
N2—Ni1—O3—S1	36.51 (10)	Ni1—N1—C1—C2	172.59 (15)
N2^{i}—Ni1—O3—S1	−143.49 (10)	C5—N1—C1—C6	179.00 (14)
N1^{i}—Ni1—O3—S1	−64.52 (10)	Ni1—N1—C1—C6	−7.13 (17)
N1—Ni1—O3—S1	115.48 (10)	N1—C1—C2—C3	0.7 (3)
O3—Ni1—N1—C5	65.02 (14)	C6—C1—C2—C3	−179.6 (2)
O3^{i}—Ni1—N1—C5	−114.98 (14)	C1—C2—C3—C4	0.2 (4)
N2—Ni1—N1—C5	158.22 (14)	C2—C3—C4—C5	−0.6 (4)
N2^{i}—Ni1—N1—C5	−21.78 (14)	C1—N1—C5—C4	0.9 (3)

N1^{i}—Ni1—N1—C5	76 (30)	Ni1—N1—C5—C4	−171.96 (16)
O3—Ni1—N1—C1	−108.16 (11)	C3—C4—C5—N1	0.0 (4)
O3^{i}—Ni1—N1—C1	71.84 (11)	C7—N2—C6—C1	81.22 (15)
N2—Ni1—N1—C1	−14.97 (11)	Ni1—N2—C6—C1	−45.48 (14)
N2^{i}—Ni1—N1—C1	165.03 (11)	N1—C1—C6—N2	36.05 (19)
N1^{i}—Ni1—N1—C1	−97 (30)	C2—C1—C6—N2	−143.67 (17)
O3—Ni1—N2—C6	121.09 (10)	C6—N2—C7—C8	−171.05 (12)
O3^{i}—Ni1—N2—C6	−58.91 (10)	Ni1—N2—C7—C8	−50.99 (15)
N2^{i}—Ni1—N2—C6	−78 (17)	N2—C7—C8—S1	83.95 (13)
N1^{i}—Ni1—N2—C6	−147.33 (9)	O2—S1—C8—C7	−166.32 (11)
N1—Ni1—N2—C6	32.67 (9)	O1—S1—C8—C7	71.88 (12)
O3—Ni1—N2—C7	−1.22 (10)	O3—S1—C8—C7	−45.17 (12)
O3^{i}—Ni1—N2—C7	178.78 (10)		

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1N···O1^{ii}	0.847 (18)	2.100 (19)	2.9394 (17)	170.6 (16)

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

Fig. 1

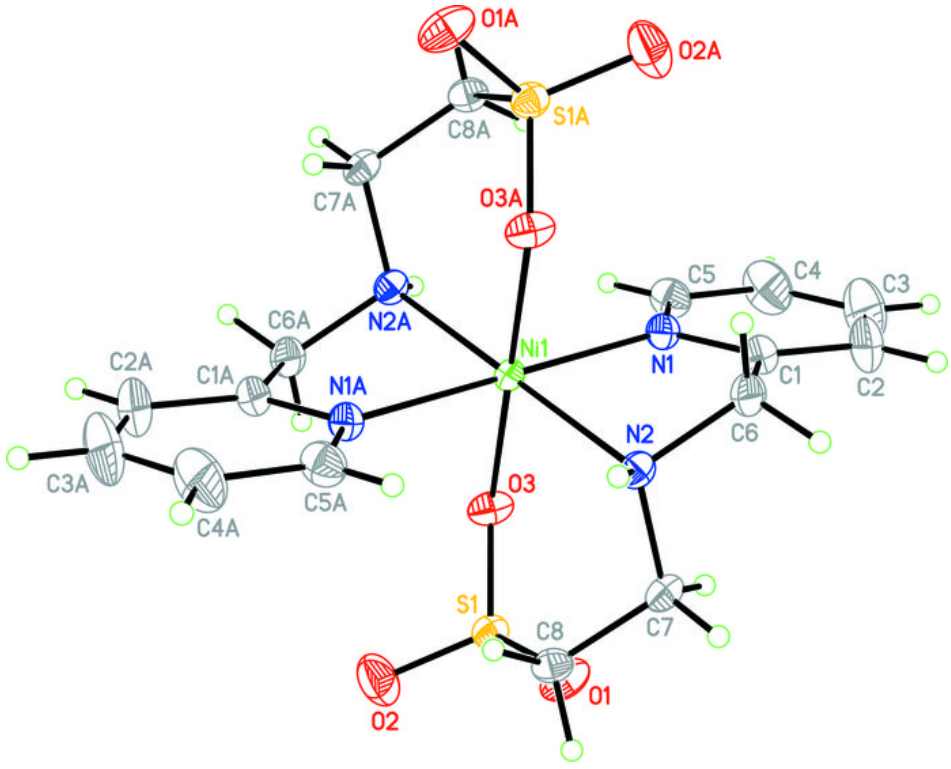
O1A
O2A
S1A
C8A
C7A
O3A
C5
C4
C3
N2A
C6A
Ni1
N1
C1
C2
C2A
C1A
N1A
N2
C6
C3A
C5A
O3
C4A
S1
C8
C7
O1
O2

Fig. 2