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Bis(*N*-butyl-*N*-ethyldithiocarbamato-$\kappa^2 S,S'$)nickel(II)

Wan Nur Shazwani Wan Juhari,[a] Ibrahim Baba,[a] Yang Farina[a] and Seik Weng Ng[b]*

[a]School of Chemical Sciences, Universiti Kebangbaan Malaysia, 43600 Bangi, Malaysia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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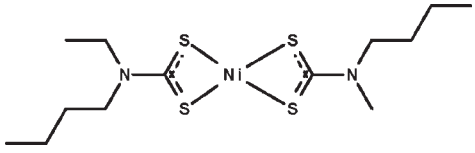
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.098; data-to-parameter ratio = 23.2.

The dithiocarbamate anions in the title compound, $[Ni(C_7H_{14}NS_2)_2]$, chelate to the Ni^{II} atom, which is four-coordinate in a square-planar geometry. The Ni^{II} atom lies on a center of inversion.

Related literature

For nickel bis(diethyldithiocarbamate) and nickel bis(dibutyldithiocarbamate), see: Bonamico *et al.* (1965); Khan *et al.* (1987); Lokaj *et al.* (1984).



Experimental

Crystal data

$[Ni(C_7H_{14}NS_2)_2]$ M_r = 411.33
Monoclinic, $P2_1/n$
a = 8.5641 (9) Å
b = 8.6316 (9) Å
c = 13.6047 (14) Å
β = 94.753 (2)°
V = 1002.23 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 293 K
0.25 × 0.25 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.724, T_{max} = 0.934
9338 measured reflections
2295 independent reflections
1628 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.098
S = 1.03
2295 reflections
99 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2734).

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supplementary materials

Acta Cryst. (2010). E**66**, m339 [**doi:10.1107/S1600536810006677**]

Bis(*N*-butyl-*N*-ethyldithiocarbamato-$\kappa^2 S,S'$)nickel(II)

W. N. S. Wan Juhari, I. Baba, Y. Farina and S. W. Ng

Experimental

Nickel(II) chloride (10 mmol), butylethylamine (10 mmol) and carbon disulfide (10 mmol) were reacted in ethanol (50 ml) at 277 K to produce a brown solid. The mixture was stirred for an hour. The solid was collected and recrystallized from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.96 to 0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C).

Figures

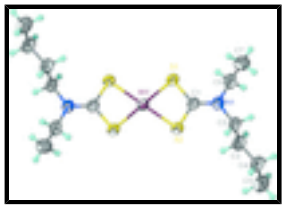

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $Ni(C_7H_{14}NS_2)_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

Bis(*N*-butyl-*N*-ethyldithiocarbamato- $\kappa^2 S,S'$)nickel(II)

Crystal data

$[Ni(C_7H_{14}NS_2)_2]$	$F(000) = 436$
$M_r = 411.33$	$D_x = 1.363$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2307 reflections
$a = 8.5641$ (9) Å	$\theta = 2.4$–$24.6°$
$b = 8.6316$ (9) Å	$\mu = 1.38$ mm^{-1}
$c = 13.6047$ (14) Å	$T = 293$ K
$\beta = 94.753$ (2)°	Plate, brown
$V = 1002.23$ (18) Å^3	0.25 × 0.25 × 0.05 mm
$Z = 2$	

Data collection

Bruker SMART APEX diffractometer	2295 independent reflections
Radiation source: fine-focus sealed tube	1628 reflections with $I > 2\sigma(I)$

graphite	R_{int} = 0.029
ω scans	θ_{max} = 27.5°, θ_{min} = 2.7°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→11
T_{min} = 0.724, T_{max} = 0.934	k = −11→11
9338 measured reflections	l = −17→15

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.034	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.098	H-atom parameters constrained
S = 1.03	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.1755P]$ where $P = (F_o^2 + 2F_c^2)/3$
2295 reflections	$(\Delta/\sigma)_{max}$ = 0.001
99 parameters	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
6 restraints	$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.5000	0.05331 (16)
S1	0.75597 (8)	0.48176 (8)	0.53089 (5)	0.0629 (2)
S2	0.52687 (8)	0.56847 (9)	0.65651 (5)	0.0631 (2)
N1	0.8339 (3)	0.5601 (3)	0.72015 (17)	0.0647 (6)
C1	0.7236 (3)	0.5403 (3)	0.64766 (19)	0.0564 (6)
C2	0.7964 (3)	0.6124 (3)	0.81795 (18)	0.0658 (7)
H2A	0.7008	0.6732	0.8111	0.079*
H2B	0.8799	0.6791	0.8456	0.079*
C3	0.7752 (4)	0.4796 (3)	0.8887 (2)	0.0746 (8)
H3A	0.6875	0.4163	0.8630	0.090*
H3B	0.8684	0.4154	0.8928	0.090*
C4	0.7460 (4)	0.5353 (4)	0.9904 (2)	0.0836 (9)
H4A	0.6554	0.6032	0.9856	0.100*
H4B	0.8355	0.5955	1.0167	0.100*
C5	0.7180 (4)	0.4044 (4)	1.0615 (2)	0.1014 (11)
H5A	0.6962	0.4470	1.1241	0.152*
H5B	0.8098	0.3403	1.0699	0.152*
H5C	0.6305	0.3433	1.0356	0.152*
C6	1.0008 (4)	0.5276 (4)	0.7074 (2)	0.0805 (9)
H6A	1.0079	0.4559	0.6530	0.097*
H6B	1.0490	0.4791	0.7667	0.097*
C7	1.0871 (4)	0.6734 (4)	0.6871 (2)	0.0951 (10)
H7A	1.1957	0.6500	0.6818	0.143*
H7B	1.0780	0.7453	0.7401	0.143*

H7C	1.0432	0.7183	0.6265	0.143*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0586 (3)	0.0553 (3)	0.0464 (3)	−0.0031 (2)	0.0063 (2)	−0.00089 (19)
S1	0.0628 (4)	0.0763 (4)	0.0504 (4)	0.0013 (3)	0.0095 (3)	−0.0089 (3)
S2	0.0589 (4)	0.0785 (5)	0.0526 (4)	0.0006 (3)	0.0090 (3)	−0.0081 (3)
N1	0.0596 (13)	0.0780 (14)	0.0572 (13)	0.0057 (11)	0.0077 (11)	−0.0171 (12)
C1	0.0629 (16)	0.0556 (14)	0.0513 (15)	−0.0005 (11)	0.0083 (12)	−0.0052 (11)
C2	0.0670 (17)	0.0758 (17)	0.0542 (16)	0.0016 (13)	0.0023 (13)	−0.0198 (13)
C3	0.080 (2)	0.080 (2)	0.0629 (18)	0.0053 (14)	0.0010 (15)	−0.0130 (15)
C4	0.093 (2)	0.096 (2)	0.0621 (19)	0.0055 (17)	0.0047 (17)	−0.0136 (17)
C5	0.118 (3)	0.111 (3)	0.074 (2)	0.001 (2)	0.002 (2)	0.000 (2)
C6	0.0653 (18)	0.109 (3)	0.0660 (19)	0.0082 (17)	−0.0034 (15)	−0.0236 (17)
C7	0.076 (2)	0.125 (3)	0.086 (2)	0.008 (2)	0.0171 (17)	−0.006 (2)

Geometric parameters (Å, °)

Ni1—S1^{i}	2.2032 (8)	C3—H3B	0.9700
Ni1—S1	2.2032 (8)	C4—C5	1.519 (4)
Ni1—S2	2.2034 (7)	C4—H4A	0.9700
Ni1—S2^{i}	2.2034 (7)	C4—H4B	0.9700
S1—C1	1.712 (3)	C5—H5A	0.9600
S2—C1	1.716 (3)	C5—H5B	0.9600
N1—C1	1.319 (3)	C5—H5C	0.9600
N1—C2	1.466 (3)	C6—C7	1.497 (4)
N1—C6	1.481 (4)	C6—H6A	0.9700
C2—C3	1.517 (4)	C6—H6B	0.9700
C2—H2A	0.9700	C7—H7A	0.9600
C2—H2B	0.9700	C7—H7B	0.9600
C3—C4	1.505 (4)	C7—H7C	0.9600
C3—H3A	0.9700		
S1^{i}—Ni1—S1	180.0	H3A—C3—H3B	107.9
S1^{i}—Ni1—S2	100.82 (2)	C3—C4—C5	113.3 (3)
S1—Ni1—S2	79.18 (2)	C3—C4—H4A	108.9
S1^{i}—Ni1—S2^{i}	79.18 (2)	C5—C4—H4A	108.9
S1—Ni1—S2^{i}	100.82 (2)	C3—C4—H4B	108.9
S2—Ni1—S2^{i}	180.0	C5—C4—H4B	108.9
C1—S1—Ni1	85.45 (10)	H4A—C4—H4B	107.7
C1—S2—Ni1	85.34 (9)	C4—C5—H5A	109.5
C1—N1—C2	121.4 (2)	C4—C5—H5B	109.5
C1—N1—C6	121.7 (2)	H5A—C5—H5B	109.5
C2—N1—C6	116.8 (2)	C4—C5—H5C	109.5
N1—C1—S1	124.8 (2)	H5A—C5—H5C	109.5
N1—C1—S2	125.1 (2)	H5B—C5—H5C	109.5
S1—C1—S2	110.04 (16)	N1—C6—C7	111.0 (3)

N1—C2—C3	113.0 (2)	N1—C6—H6A	109.4
N1—C2—H2A	109.0	C7—C6—H6A	109.4
C3—C2—H2A	109.0	N1—C6—H6B	109.4
N1—C2—H2B	109.0	C7—C6—H6B	109.4
C3—C2—H2B	109.0	H6A—C6—H6B	108.0
H2A—C2—H2B	107.8	C6—C7—H7A	109.5
C4—C3—C2	112.3 (2)	C6—C7—H7B	109.5
C4—C3—H3A	109.1	H7A—C7—H7B	109.5
C2—C3—H3A	109.1	C6—C7—H7C	109.5
C4—C3—H3B	109.1	H7A—C7—H7C	109.5
C2—C3—H3B	109.1	H7B—C7—H7C	109.5
S2—Ni1—S1—C1	−0.24 (9)	Ni1—S1—C1—S2	0.32 (12)
$S2^{i}$—Ni1—S1—C1	179.76 (9)	Ni1—S2—C1—N1	180.0 (2)
$S1^{i}$—Ni1—S2—C1	−179.76 (9)	Ni1—S2—C1—S1	−0.32 (12)
S1—Ni1—S2—C1	0.24 (9)	C1—N1—C2—C3	94.2 (3)
C2—N1—C1—S1	179.3 (2)	C6—N1—C2—C3	−84.6 (3)
C6—N1—C1—S1	−2.0 (4)	N1—C2—C3—C4	176.7 (3)
C2—N1—C1—S2	−1.0 (4)	C2—C3—C4—C5	177.8 (3)
C6—N1—C1—S2	177.6 (2)	C1—N1—C6—C7	98.5 (3)
Ni1—S1—C1—N1	−180.0 (2)	C2—N1—C6—C7	−82.8 (3)

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

Fig. 1