Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $U_{eq}$ |
|---|---|---|---|---|
| S | 0.44178 (5) | 0.85943 (6) | 0.21876 (10) | 0.0333 (2) |
| N | 1/2 | 0.6607 (3) | 1/4 | 0.0247 (7) |
| C1 | 0.4349 (2) | 0.7184 (2) | 0.2185 (3) | 0.0248 (6) |
| C2 | 0.3575 (2) | 0.6696 (3) | 0.1843 (4) | 0.0333 (7) |
| C3 | 0.3008 (2) | 0.7322 (4) | 0.2318 (5) | 0.0488 (9) |
| C4 | 0.2285 (2) | 0.6907 (4) | 0.2097 (6) | 0.0571 (11) |
| C5 | 0.2113 (2) | 0.5880 (4) | 0.1390 (5) | 0.0538 (11) |
| C6 | 0.2630 (2) | 0.5265 (4) | 0.0890 (5) | 0.0530 (10) |
| C7 | 0.3395 (2) | 0.5669 (3) | 0.1116 (4) | 0.0421 (8) |
| C8 | 0.3934 (2) | 0.4999 (3) | 0.0540 (5) | 0.0498 (9) |
| As | 1/2 | 0.18651 (4) | 1/4 | 0.0315 (2) |
| F1 | 0.4085 (2) | 0.1852 (3) | 0.1079 (3) | 0.0795 (9) |
| F2 | 0.5278 (2) | 0.2834 (2) | 0.1353 (3) | 0.0674 (8) |
| F3 | 0.5275 (2) | 0.0871 (2) | 0.1369 (3) | 0.0571 (6) |

Table 2. *Selected geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S—C1 | 1.724 (3) | N···F2$^{iii}$ | 3.207 (7) |
| S—S$^{i}$ | 2.004 (2) | S···F3$^{iv}$ | 3.011 (6) |
| N—C1 | 1.326 (3) | S···F3$^{ii}$ | 3.297 (6) |
| C1—C2 | 1.465 (4) | S···F3$^{v}$ | 3.361 (6) |
| As—F2 | 1.704 (2) | S···F3$^{iii}$ | 3.436 (6) |
| As—F1 | 1.706 (3) | S···F1$^{iii}$ | 3.575 (6) |
| As—F3 | 1.715 (2) | S···F2$^{ii}$ | 3.657 (6) |
| N···F2$^{ii}$ | 3.207 (7) | | |
| C1—S—S$^{i}$ | 94.04 (10) | N—C1—S | 118.0 (2) |
| C1$^{i}$—N—C1 | 115.8 (4) | C2—C1—S | 118.1 (2) |
| N—C1—C2 | 123.9 (3) | | |

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

H atoms were placed geometrically and refined using a riding model with $U_{iso}$ constrained to be 1.2 (1.5 for methyl groups) times $U_{eq}$ of the carrier atom. This produces no additional refined parameters except for the torsional freedom of the methyl group about the C—C bond.

Data collection: *DIF*4 (Stoe & Cie, 1988). Cell refinement: *DIF*4. Data reduction: local programs. Program(s) used to solve structure: *SHELXTL* (Sheldrick, 1994). Program(s) used to refine structure: *SHELXTL*. Molecular graphics: *SHELXTL*. Software used to prepare material for publication: *SHELXTL* and local programs.

We thank EPSRC for financial support.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: BK1238). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1996). C**52**, 2150–2153

# Bis[methyl $N^{\beta}$-(4-dimethylaminophenylmethylene)dithiocarbazato]nickel(II)

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(*Received 1 November 1995; accepted 18 March 1996*)

## Abstract

There are two independent centrosymmetric and essentially planar molecules in the unit cell of the title compound, $[Ni(C_{11}H_{14}N_3S_2)_2]$, having slightly different ligand conformations and a square-planar coordination of the Ni atom. Within each molecule, the two ligands are linked by a pair of C—H···S hydrogen-bonding interactions.

## Comment

Metal complexes of chelating agents derived from dithiocarbazic acid are of considerable interest (West, Liberta, Padhye, Chikate, Sonawane, Kumbhar & Yerande, 1993). The thio derivatives of Schiff bases,

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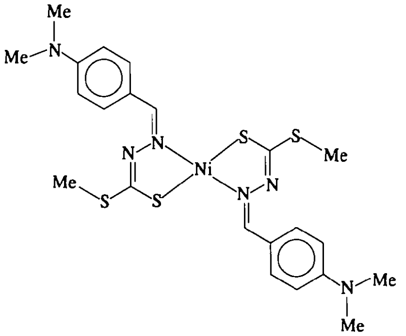
*R*CH=NNHCSS*R*′, are known to coordinate readily with transition metals to give stable complexes of which some have been shown to possess biological activity (Scovill, Klayman, Lambros, Childs & Notsch, 1984) or nonlinear optical properties (Zhao, Samoc, Singh & Prasad, 1989). We have synthesized a series of Schiff base thio derivatives and their metal complexes in order to study their potential nonlinear optical properties. In the present paper, we report the X-ray structure determination of one of these compounds, namely, bis[methyl $N^{\beta}$-(4-dimethylaminophenylmethylene)dithiocarbazato]nickel(II), (I).



(I)

The structure contains two crystallographically independent centrosymmetric molecules (Fig. 1), the asymmetric unit consisting of two half molecules, as found previously for the related complex bis[methyl $N^{\beta}$-(4-methoxyphenylmethylene)dithiocarbazato]nickel(II) (Fun, Sivakumar, Tian, Duan, Lu & You, 1996). In both molecules, the Ni atom is coordinated in a distorted *trans* square-planar configuration, the distortion consisting of a reduction of the N—Ni—S angle within the chelate rings from the ideal value of 90°. Bond lengths and angles in the two molecules (*A* and *B*) are similar, but there are some differences in the torsion angles of the chelate rings. The ligands are essentially planar, with a larger deviation in molecule *A* [maximum of 0.243 (3) Å for N1*A*] than in molecule *B* [maximum of 0.135 (2) Å for N2*B*]. The dihedral angle between the mean planes of the two molecules is 74.34 (2)°.

Intramolecular C—H···S hydrogen-bonding interactions exist between the two ligands of each molecule as indicated by the geometric parameters; H2*A*···S1*A*$^{i}$ 2.50 (3), C2*A*···S1*A*$^{i}$ 3.063 (3) Å, C2*A*—H2*A*···S1*A*$^{i}$ 121 (2)°, and H2*B*···S1*B*$^{ii}$ 2.46 (3), C2*B*···S1*B*$^{ii}$ 3.061 (3) Å, C2*B*—H2*B*···S1*B*$^{ii}$ 125 (2)° [symmetry codes: (i) $-x+1$, $-y+1$, $-z$; (ii) $-x$, $-y$, $-z+1$]. Similar interactions have been observed in other structures of this family (Uechi & Oniki, 1982; Fun *et al.*, 1996). There are no particularly close intermolecular contacts, the shortest Ni···S distances being 4.614 (1) Å between molecules of *A* and 3.754 (1) Å between molecules of *B*, the molecules of each type being stacked parallel in columns along the *a* axis.

## Experimental

The title complex was prepared by refluxing a mixture of the ethanol solutions of the ligand methyl $N^{\beta}$-(4-dimethylaminophenylmethylene)dithiocarbazate and nickel acetate for 4 h. Single crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane/2-propanol solution of the complex.

*Crystal data*

$[Ni(C_{11}H_{14}N_3S_2)_2]$
$M_r = 563.45$
Triclinic
$P\overline{1}$
$a = 5.7712$ (3) Å
$b = 10.513$ (1) Å
$c = 21.633$ (2) Å
$\alpha = 94.09$ (1)°
$\beta = 90.114$ (6)°
$\gamma = 105.871$ (6)°
$V = 1259.0$ (2) Å$^3$
$Z = 2$
$D_x = 1.486$ Mg m$^{-3}$

Mo *Kα* radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 8$–25°
$\mu = 1.126$ mm$^{-1}$
$T = 293$ (2) K
Prism
0.42 × 0.34 × 0.16 mm
Black

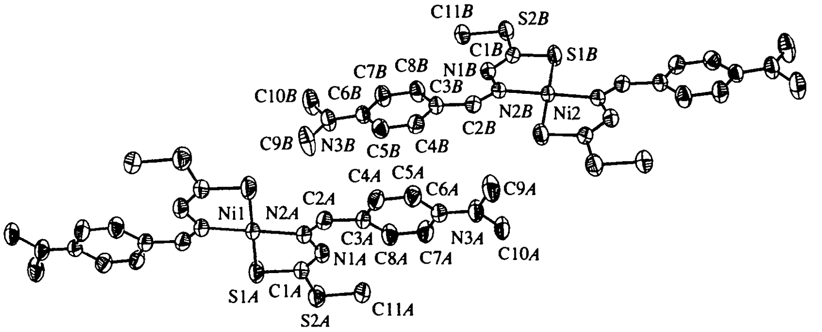


Fig. 1. Perspective plot of the title molecule with the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

*Data collection*

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
5837 measured reflections
4419 independent reflections
3337 observed reflections [$I > 2\sigma(I)$]
$R_{\rm int} = 0.0252$
$\theta_{\rm max} = 25°$
$h = -1 \rightarrow 6$
$k = -12 \rightarrow 12$
$l = -25 \rightarrow 25$
3 standard reflections monitored every 97 reflections intensity decay: <3%

*Refinement*

Refinement on $F^2$
$R(F) = 0.0388$
$wR(F^2) = 0.1002$
$S = 0.938$
4419 reflections
413 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.407$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.572$ e Å$^{-3}$
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å$^2$)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $U_{\rm eq}$ |
|---|---|---|---|---|
| Ni1 | 1/2 | 1/2 | 0 | 0.0450 (2) |
| S1*A* | 0.3287 (2) | 0.66026 (9) | 0.00613 (4) | 0.0709 (3) |
| S2*A* | 0.1115 (2) | 0.76503 (9) | 0.11273 (4) | 0.0624 (2) |
| N1*A* | 0.3600 (5) | 0.5886 (2) | 0.12095 (11) | 0.0485 (6) |
| N2*A* | 0.4964 (5) | 0.5138 (2) | 0.08897 (11) | 0.0463 (6) |
| N3*A* | 0.7709 (5) | 0.4256 (3) | 0.38027 (11) | 0.0535 (7) |
| C1*A* | 0.2788 (6) | 0.6579 (3) | 0.08464 (13) | 0.0474 (7) |
| C2*A* | 0.6188 (6) | 0.4599 (3) | 0.12454 (14) | 0.0475 (7) |
| C3*A* | 0.6393 (6) | 0.4563 (3) | 0.19089 (12) | 0.0451 (7) |
| C4*A* | 0.7911 (6) | 0.3843 (3) | 0.21127 (14) | 0.0516 (8) |
| C5*A* | 0.8340 (7) | 0.3712 (3) | 0.27244 (14) | 0.0526 (8) |
| C6*A* | 0.7243 (5) | 0.4329 (3) | 0.31897 (13) | 0.0429 (7) |
| C7*A* | 0.5687 (6) | 0.5035 (3) | 0.29920 (14) | 0.0537 (8) |
| C8*A* | 0.5248 (6) | 0.5148 (3) | 0.23760 (14) | 0.0526 (8) |
| C9*A* | 0.9170 (9) | 0.3442 (5) | 0.3999 (2) | 0.0686 (12) |
| C10*A* | 0.6619 (8) | 0.4902 (4) | 0.4281 (2) | 0.0573 (9) |
| C11*A* | 0.1228 (9) | 0.7513 (4) | 0.1949 (2) | 0.0654 (10) |
| Ni2 | 0 | 0 | 1/2 | 0.0396 (2) |
| S1*B* | −0.3322 (2) | −0.15275 (8) | 0.51329 (4) | 0.0576 (2) |
| S2*B* | −0.7378 (2) | −0.26366 (8) | 0.42787 (4) | 0.0554 (2) |
| N1*B* | −0.3343 (4) | −0.0945 (2) | 0.39488 (10) | 0.0435 (6) |
| N2*B* | −0.1012 (4) | −0.0167 (2) | 0.41388 (10) | 0.0417 (5) |
| N3*B* | −0.0760 (5) | 0.0920 (3) | 0.11335 (11) | 0.0541 (7) |
| C1*B* | −0.4466 (5) | −0.1584 (3) | 0.43960 (12) | 0.0418 (6) |
| C2*B* | 0.0295 (6) | 0.0376 (3) | 0.36920 (13) | 0.0432 (7) |
| C3*B* | −0.0146 (5) | 0.0405 (3) | 0.30361 (12) | 0.0407 (6) |
| C4*B* | 0.1792 (6) | 0.1117 (3) | 0.27022 (13) | 0.0462 (7) |
| C5*B* | 0.1627 (6) | 0.1273 (3) | 0.20794 (14) | 0.0490 (7) |
| C6*B* | −0.0547 (5) | 0.0727 (3) | 0.17443 (13) | 0.0437 (7) |
| C7*B* | −0.2474 (6) | 0.0001 (3) | 0.20747 (14) | 0.0537 (8) |
| C8*B* | −0.2301 (6) | −0.0162 (4) | 0.26950 (15) | 0.0537 (8) |
| C9*B* | 0.1193 (9) | 0.1718 (6) | 0.0801 (2) | 0.0799 (14) |
| C10*B* | −0.2877 (9) | 0.0211 (6) | 0.0769 (2) | 0.0764 (12) |
| C11*B* | −0.7985 (8) | −0.2521 (4) | 0.3474 (2) | 0.0610 (9) |

Table 2. *Selected geometric parameters (Å, °)*

| | Molecule *A* | Molecule *B* |
|---|---|---|
| Ni—N2 | 1.920 (2) | 1.933 (2) |
| Ni—S1 | 2.171 (1) | 2.173 (1) |
| S1—C1 | 1.724 (3) | 1.715 (3) |
| S2—C1 | 1.752 (3) | 1.748 (3) |
| S2—C11 | 1.795 (4) | 1.794 (3) |
| N1—C1 | 1.279 (4) | 1.290 (4) |
| N1—N2 | 1.407 (4) | 1.413 (3) |
| N2—C2 | 1.300 (4) | 1.294 (4) |
| N3—C6 | 1.364 (4) | 1.361 (3) |
| N3—C9 | 1.438 (5) | 1.437 (5) |
| N3—C10 | 1.436 (4) | 1.444 (5) |
| C2—C3 | 1.444 (4) | 1.445 (4) |
| C3—C4 | 1.394 (4) | 1.399 (4) |
| C3—C8 | 1.405 (4) | 1.405 (4) |
| C4—C5 | 1.369 (4) | 1.375 (4) |
| C5—C6 | 1.403 (4) | 1.404 (4) |
| C6—C7 | 1.396 (4) | 1.395 (4) |
| C7—C8 | 1.376 (4) | 1.372 (4) |
| N2—Ni—S1 | 85.3 (1) | 85.9 (1) |
| C1—S1—Ni | 96.0 (1) | 96.1 (1) |
| C1—S2—C11 | 102.2 (2) | 103.0 (2) |
| C1—N1—N2 | 111.6 (2) | 111.6 (2) |
| C2—N2—N1 | 114.5 (2) | 114.1 (2) |
| C2—N2—Ni | 124.6 (2) | 125.5 (2) |
| N1—N2—Ni | 120.9 (2) | 120.4 (2) |
| C6—N3—C9 | 121.2 (3) | 122.1 (3) |
| C6—N3—C10 | 121.7 (3) | 121.3 (3) |
| C9—N3—C10 | 116.9 (3) | 116.2 (3) |
| N1—C1—S1 | 124.6 (3) | 125.3 (2) |
| N1—C1—S2 | 121.3 (2) | 120.6 (2) |
| S1—C1—S2 | 114.1 (2) | 114.0 (2) |
| N2—C2—C3 | 133.5 (3) | 133.7 (3) |
| C4—C3—C8 | 115.7 (3) | 115.9 (3) |
| C4—C3—C2 | 115.8 (3) | 116.0 (3) |
| C8—C3—C2 | 128.5 (3) | 128.1 (3) |
| C5—C4—C3 | 123.8 (3) | 122.8 (3) |
| C4—C5—C6 | 120.2 (3) | 121.0 (3) |
| N3—C6—C7 | 122.0 (3) | 122.2 (3) |
| N3—C6—C5 | 121.4 (3) | 121.5 (3) |
| C7—C6—C5 | 116.6 (3) | 116.3 (3) |
| C8—C7—C6 | 122.7 (3) | 122.6 (3) |
| C7—C8—C3 | 120.9 (3) | 121.3 (3) |
| C1—N1—N2—C2 | 168.3 (3) | 172.5 (3) |
| N2—N1—C1—S1 | 0.1 (4) | −0.3 (4) |
| N2—N1—C1—S2 | −177.7 (2) | −179.2 (2) |
| C11—S2—C1—N1 | 4.1 (3) | 1.1 (3) |
| C11—S2—C1—S1 | −173.9 (21) | −177.9 (2) |
| N1—N2—C2—C3 | 2.5 (5) | 3.0 (5) |
| N2—C2—C3—C4 | −179.0 (3) | −179.8 (3) |
| N2—C2—C3—C8 | −0.3 (6) | 2.3 (6) |

The title structure was solved by direct methods. The H atoms were located from difference maps and refined freely with individual $U_{\rm iso}$ values.

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC*. Molecular geometry: *PARST* (Nardelli, 1983). Software used to prepare material for publication: *SHELXL93*.

The authors would like to thank the State Science and Technology Commission and National Nature Science Foundation of China for a major key research project and the Malaysian Government and Universiti Sains Malaysia for research grant R & D No. 123-3417-2201. KS thanks Universiti Sains Malaysia for a Visiting Post Doctoral Research Fellowship.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: CF1065). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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*Acta Cryst.* (1996). C**52**, 2153–2155

# 1,4-Dimethylpyridinium Bis(6,7-dihydro-5*H*-1,4-dithiepine-2,3-dithiolato-*S*,*S*′)cuprate(III)

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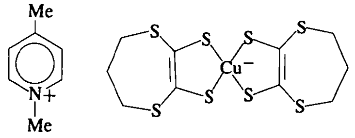
(*Received 13 February 1996; accepted 14 March 1996*)

## Abstract

In the title complex, $(C_7H_{10}N)[Cu(C_5H_6S_4)_2]$, the $CuS_4$ core adopts a square-planar geometry. Alternate columns of cations and anions form thick layers parallel to the *bc* plane. Weak C—H···Cu and C—H···S interactions help to link the cations and anions together.

## Comment

Ever since the metal complexes of 4,5-dimercapto-1,3-dithiole-2-thionate (dmit) were first reported to exhibit high conductivities, a massive research effort has centred on the design and synthesis of similar complexes (Cassoux, Valade, Kobayashi, Kobayashi, Clark & Underhill, 1991). The multi-sulfur 1,2-dithiolene complexes $[M(dddt)_2]^-$ ($M$ = Cu, Ni; dddt = 6,7-dihydro-5*H*-1,4-dithiepine-2,3-dithiolate) have been synthesized and studied previously (Bereman & Lu, 1993; Yao, You, Li, Li & Yang, 1994). It is believed that molecular interactions through S···S contacts form effective electrical conduction pathways in these crystal phases. In addition, the introduction of various organic counter cations is of interest because of the possibilities of modifying the interactions between the anions (Cornelissen, Creyghton, de Graaff, Haasnoot & Reedijk, 1991). In order to investigate the effects of the cation on the crystal packing and properties, the title complex, (I), was prepared for comparison with $(Bu_4N)[Cu(dddt)_2]$ and $(Et_4N)[Cu(dddt)_2]$.



(I)

The crystal of (I) is built from exactly centrosymmetric cations and anions (Fig. 1). The former are disordered and there is an equal probability that the sites labelled C7 and N7 in Fig. 1 contain C or N atoms. The four S atoms surround the Cu atom yielding a square-planar environment, with nearly equal Cu—S bond lengths and S—Cu—S bond angles. In the five-membered ring containing the Cu atom, the average Cu—S, S—C and C═C bond lengths are 2.184 (1), 1.747 (3) and 1.339 (4) Å, respectively. The corresponding values in $(Bu_4N)[Cu(dddt)_2]$ are 2.181, 1.749 and 1.342 Å, and in $(Et_4N)[Cu(dddt)_2]$ are 2.182, 1.749 and 1.337 Å. The seven-membered ring (S3, C3–C5, S4, C2, C1) adopts a chair conformation. The anion as a whole has an extended linear conformation. The cation is planar and makes an angle of 69.4 (1)° with the plane of the anion.

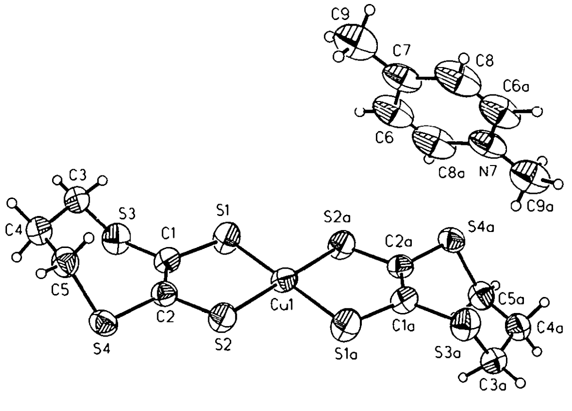


Fig. 1. A 50% probability displacement ellipsoid plot of the title compound with the atom-numbering scheme. The disorder of the C7/N7 site is not shown.

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