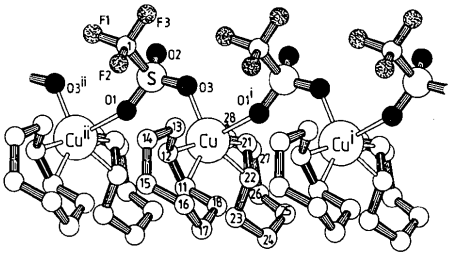

Fig. 1. *PLUTO* drawing showing three units of the chain structure of CuOTf(cyclooctene)$_2$ with the adopted numbering scheme.

with the longer S–O bonds corresponding to Cu–O interactions; bridging triflate anions have also been found in CuOTf(benzene)$_{1/2}$ (Dines & Bird, 1973). The cyclooctene ligands have a boat-twist conformation and are nearly each other's mirror images (*cf.* the torsion angles in Table 2).

The most interesting aspect of the present structure is the copper–olefin interaction. The distances from Cu to the midpoints of the two double bonds are nearly equal (2·05 Å ave.), although one of the two π bonds is coordinated somewhat asymmetrically (see Table 2). According to *ab initio* calculations (Merchan, Gonzalez-Luque, Nebot-Gil & Tomas, 1984) such a deformation from the ideal geometry costs very little energy; thus, it may simply be caused by packing forces here. Values for the Cu^{I}–olefin bond lengths reported to date have been deposited. They are seen to vary over a range of 1·88–2·2 Å, and the present complex fits in at the upper part of the range. As far as it is possible to generalize from this limited set of data, it appears that bis(olefin)copper(I) complexes have longer Cu–olefin bonds than mono(olefin) complexes. In accord with this, CuOTf(cyclooctene)$_2$ easily loses one molecule of cyclooctene, but the last molecule is retained tenaciously. Tris(olefin)copper(I) complexes are probably only isolable for very strongly coordinating olefins.

This work was supported in part by the Netherlands Foundation for Chemical Research (SON) with financial aid from the Netherlands Organization for the Advancement of Pure Research (ZWO).

References

BAENZIGER, N. C., RICHARDS, G. F. & DOYLE, J. R. (1964). *Inorg. Chem.* **3**, 1529–1535.

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

CROMER, D. T. & MANN, J. B. (1968). *Acta Cryst.* A**24**, 321–324.

DINES, M. B. & BIRD, P. H. (1973). *J. Chem. Soc. Chem. Commun.* p. 12.

EVERS, J. TH. (1979). PhD Thesis, Utrecht, The Netherlands.

GANIS, P., LEPORE, U. & MARTUSCELLI, E. (1970). *J. Phys. Chem.* **74**, 2439–2444.

HENNIG, H., REHOREK, D. & ARCHER, R. D. (1985). *Coord. Chem. Rev.* **61**, 1–53.

KROPP, P. J. (1979). *Org. Photochem.* **4**, 1–142.

MERCHAN, M., GONZALEZ-LUQUE, R., NEBOT-GIL, I. & TOMAS, F. (1984). *Chem. Phys. Lett.* **112**, 412–416.

MOGGI, L., JURIS, A., SANDRINI, D. & MANFRIN, M. F. (1981). *Rev. Chem. Intermediates*, **4**, 171–223.

MOGGI, L., JURIS, A., SANDRINI, D. & MANFRIN, M. F. (1984). *Rev. Chem. Intermediates*, **5**, 107–155.

SALOMON, R. G. (1983). *Tetrahedron*, **39**, 485–575.

SHELDRICK, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

SPEK, A. L. (1982). *The EUCLID Package.* In *Computational Crystallography*, edited by D. SAYRE, p. 528. Oxford: Clarendon Press.

TIMMERMANS, P. J. J. A., MACKOR, A., SPEK, A. L. & KOJIĆ-PRODIĆ, B. (1984). *J. Organomet. Chem.* **276**, 287–295.

VAN DEN HENDE, J. H. & BAIRD, W. C. JR (1963). *J. Am. Chem. Soc.* **85**, 1009–1010.

Acta Cryst. (1987). C**43**, 2300–2303

Structures of Catalytically Related Species Involving Copper(II) Halides. IV. Bis(2,6-diamino-3,5-dichloropyridinium) Tetrachlorocuprate(II)

BY ROGER D. WILLETT

Department of Chemistry, Washington State University, Pullman, WA 99164–4630, *USA*

AND DOUGLAS X. WEST

Department of Chemistry, Illinois State University, Normal, IL 61761, *USA*

(*Received* 9 *March* 1987; *accepted* 7 *July* 1987)

Abstract. $2C_5H_6Cl_2N_3^+.CuCl_4^{2-}$, $M_r = 563{\cdot}4$, monoclinic, $P2_1/c$, $a = 8{\cdot}931\ (4)$, $b = 13{\cdot}584\ (7)$, $c = 16{\cdot}054\ (5)$ Å, $\beta = 92{\cdot}77\ (3)°$, $V = 1945\ (1)$ Å^3, $Z = 4$, $D_x = 1{\cdot}92$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 22{\cdot}6$ cm^{-1}, $F(000) = 1116$, $T = 295$ K, $R = 0{\cdot}040$ for 2056 unique observed reflections with $F \geq 3\sigma(F)$. The

0108-2701/87/122300-04$01.50

structure consists of the substituted pyridinium cations and distorted $CuCl_4^{2-}$ anions. The dichlorinated pyridinium cations were formed by the catalytic action of copper(II) chloride upon the parent 2,6-diaminopyridinium cation. The two independent cations are essentially identical. The ring C—N bonds average 1·355 (8) Å, while the external C—N bonds are slightly shorter at 1·337 (9) Å. The C—Cl bonds average 1·727 (6) Å. The $CuCl_4^{2-}$ anion assumes an intermediate geometry between square planar and tetrahedral, with nearly D_{2d} symmetry. The Cu—Cl bonds average 2·263 (5) Å with *trans* Cl—Cu—Cl bond angles averaging 156·6 (6)°.

Introduction. Copper halides are known to catalyze a variety of organic reactions (Lockhart, 1983; Ng & Leung, 1981). The oxidation and polymerization of phenols is catalyzed by copper(I) chloride and pyridine in methanol (Hay, Blanchard, Endres & Eustance, 1959; Finkbeiner, Hay, Blanchard & Endres, 1966) and the active species has been identified as $Cu_2Cl_2(OH)(OCH_3)py_2$ (Davies & El-Sayed, 1983). The crystal structure of the corresponding bis(methoxide) complex has been determined (Willett & Breneman, 1983), as well as the phenoxide precursor (Marengo-Rullàn & Willett, 1986). This system plays a role model for copper-oxidase activity (Jameson & Blackburn, 1975). Reactions involving tertiary amines have been shown to proceed *via* a free-radical mechanism (Zhelyazkova, 1981). Copper alkyl halides also prove to be effective in dimerization of primary alkyl groups (Tamura & Kochi, 1971). We have observed a number of instances where copper(II) bromides have shown different types of reactivity. Salts crystallized from organic solvents frequently show a precipitate of an insoluble copper(I) bromide upon redissolution in water, which rapidly reoxidizes to copper(II) in the presence of dissolved O_2. In our studies of copper(II) halide salts of substituted pyridinium ions, we have observed the bromination of 2-amino-*n*-methylpyridinium rings ($n = 3$ or 6) (Place & Willett, 1987; Grigereit, Ramakrishna, Place, Willett, Pellacani, Manfredini, Menabue, Bonamartini-Corradi & Battaglia, 1987). In this paper, the crystal structure of the reaction product obtained from the reaction of 2,6-diaminopyridine with $CuCl_2.2H_2O$ in dilute HCl is reported.

Experimental. The salt was prepared by refluxing a 2:1 mole ratio of 2,6-diaminopyridine and $CuCl_2.2H_2O$ in an equal volume HCl/ethanol solution. Crystals were grown by slow evaporation of a dilute HCl solution. Yellow crystal 0·20 × 0·25 × 0·10 mm. Nicolet $P2_1$ diffractometer upgraded to *P3F* specifications. Cell dimensions from 25 reflections with $27 < 2\theta < 35°$. 2692 measured reflections, 2524 unique reflections, 1° ω scan, variable speed, 3·9° min^{-1} minimum, 29·3° min^{-1} maximum, $2\theta_{max} = 45°$, $0 \le h \le 9$, $0 \le k \le 14$, $-16 \le l \le 16$, $R_{int} = 0·022$. Two standard reflections (212, 23$\bar{3}$) measured every 100 reflections; variations within statistical fluctuations (Campana, Shepherd & Litchman, 1981). Empirical absorption corrections assuming ellipsoidally shaped crystal, transmission factors 0·711 minimum, 0·972 maximum. Cu and Cl positions *via* direct methods with *SHELXTL* package (Sheldrick, 1986) on a Data General Eclipse S140/E computer. Remaining atoms from resulting difference syntheses. Least-squares refinement on F^2 for 2056 observed reflections [$F \ge 3\sigma(F)$] with anisotropic thermal parameters for non-H atoms. H atoms were located on difference maps and their locations constrained to C—H and N—H distances of 0·96 Å and isotropic thermal parameters fixed at $U = 0·06$ Å^2 (amino groups) or at approximately 20% larger than the corresponding heavy-atom parameter. $R = 0·040$, $wR = 0·037$, $w = 1/[\sigma^2(F) + g|F|^2]$, $g = 0·0009$. 226 parameters. $|\Delta/\sigma_{max}| = 0·04$. Goodness of fit = 1·514. $\Delta\rho_{max} = 0·3$ e Å^{-3} near Cu. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).*

Discussion. Atomic parameters are given in Table 1. The crystal contains substituted pyridinium cations and $CuCl_4^{2-}$ anions. Hydrogen bonding (Fig. 1 and Table 2*c*) between the pyridinium protons and the chloride ions provides lattice stability. The amino groups activate the *para* positions for halide substitution, and thus the Cl atoms occupy the 3 and 5 positions of the pyridinium ring. Similar *para* activation in monosubstituted aminopyridinium cations (Place & Willett, 1987; Grigereit *et al.*, 1987) was previously observed. However, halide substitution of the monoaminopyridinium ions occurred only in the presence of copper(II) bromide. The increased activation of the ring system for the 2,6-diaminopyridinium cation allows for the chlorine substitution. The geometries of the two crystallographically independent cations (Fig. 1 and Table 2) are essentially identical. The ring C—N distances, 1·355 (8) Å average, are somewhat shorter than the ring C—C distances, 1·382 (8) Å. This leads to distortion of the ring system with the N(ring)—C—N(external) angles less than 120° [117·2 (7)° average] and both the C—N(ring)—C and the N(external)—C—C angles much larger than 120° [125·4 (6) and 125·9 (6)° averages, respectively]. The least-squares planes of both pyridinium cations are nearly normal to the crystallographic *b* axis, forming stacks along the *b* axis.

* Anisotropic thermal parameters, H-atom positions, a stereoview and a listing of observed and calculated stucture factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44262 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *for* $[C_5H_6Cl_2N_3]_2[CuCl_4]$

The equivalent isotropic U is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cu	7668 (1)	1767 (1)	8310 (1)	34 (1)
Cl(1)	9107 (2)	493 (1)	7863 (1)	50 (1)
Cl(2)	6019 (1)	679 (1)	8804 (1)	45 (1)
Cl(3)	6927 (2)	2975 (1)	9178 (1)	44 (1)
Cl(4)	8582 (2)	2803 (1)	7384 (1)	53 (1)
C(1)	2431 (5)	1306 (4)	−138 (3)	37 (2)
C(2)	1398 (5)	1421 (3)	495 (3)	33 (2)
C(3)	1908 (5)	1685 (3)	1288 (3)	36 (2)
C(4)	3397 (5)	1848 (3)	1474 (3)	36 (2)
C(5)	4416 (5)	1746 (3)	852 (3)	34 (2)
N(6)	3873 (4)	1495 (3)	79 (3)	36 (2)
N(7)	2079 (5)	1044 (3)	−914 (3)	43 (2)
Cl(8)	−473 (2)	1223 (1)	240 (1)	53 (1)
Cl(9)	4066 (2)	2150 (1)	2465 (1)	55 (1)
N(10)	5914 (4)	1851 (3)	951 (3)	47 (2)
C(11)	2873 (6)	416 (4)	6679 (3)	37 (2)
C(12)	3912 (5)	647 (4)	6099 (3)	37 (2)
C(13)	3439 (6)	967 (3)	5316 (3)	37 (2)
C(14)	1950 (6)	1098 (4)	5114 (3)	36 (2)
C(15)	896 (5)	956 (4)	5705 (3)	36 (2)
N(16)	1414 (5)	607 (3)	6462 (3)	39 (2)
N(17)	3171 (5)	56 (3)	7448 (3)	47 (2)
Cl(18)	5786 (2)	468 (1)	6384 (1)	56 (1)
Cl(19)	1311 (2)	1459 (1)	4125 (1)	55 (1)
N(20)	−585 (4)	1102 (3)	5600 (3)	47 (2)

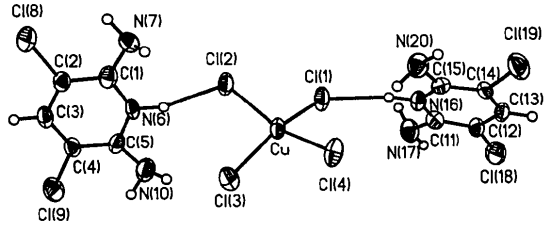

Fig. 1. View of the asymmetric unit of $[C_5H_6Cl_2N_3]_2[CuCl_4]$.

The $CuCl_4^{2-}$ anion assumes a geometry intermediate between tetrahedral and square planar. The *trans* Cl–Cu–Cl angles are relatively large, with Cl(1)–Cu–Cl(3) = 157·2 (1)° and Cl(2)–Cu–Cl(4) = 156·0 (1)°. These values typically range from 130° for large, bulky, non-hydrogen-bonding cations to 180° (planar) for cations which are capable of forming many hydrogen bonds (Smith, 1976). This is rationalized in terms of charge-compensation effects where, in the absence of hydrogen bonding, electrostatic repulsions between the chloride ions force a nearly tetrahedral geometry. Hydrogen bonding removes charge from the chloride ions, allowing the anion to relax back towards the square-planar configuration favored by crystal-field effects (Willett & Geiser, 1984). The distortion observed is consistent with these observations.

This work was supported by NSF grants DMR-8219430 and INT-8219425. The X-ray diffraction facility was established through grants from the National Science Foundation (CHE-8408407) and The Boeing Company.

Table 2. *Molecular geometry for* $[C_5H_6Cl_2N_3]_2[CuCl_4]$

(*a*) Bond lengths (Å)

Cu–Cl(1)	2·292 (2)	Cu–Cl(2)	2·257 (1)
Cu–Cl(3)	2·272 (1)	Cu–Cl(4)	2·230 (2)
C(1)–C(2)	1·413 (7)	C(1)–N(6)	1·342 (6)
C(1)–N(7)	1·320 (6)	C(2)–C(3)	1·379 (7)
C(2)–Cl(8)	1·722 (5)	C(3)–C(4)	1·366 (7)
C(4)–C(5)	1·390 (7)	C(4)–Cl(9)	1·723 (5)
C(5)–N(6)	1·355 (6)	C(5)–N(10)	1·347 (6)
C(11)–C(12)	1·383 (7)	C(11)–N(16)	1·358 (6)
C(11)–N(17)	1·341 (7)	C(12)–C(13)	1·377 (7)
C(12)–Cl(18)	1·730 (5)	C(13)–C(14)	1·365 (7)
C(14)–C(15)	1·383 (7)	C(14)–Cl(19)	1·732 (5)
C(15)–N(16)	1·364 (7)	C(15)–N(20)	1·340 (6)

(*b*) Bond angles (°)

Cl(1)–Cu–Cl(2)	90·1 (1)	Cl(1)–Cu–Cl(3)	157·2 (1)
Cl(2)–Cu–Cl(3)	92·5 (1)	Cl(1)–Cu–Cl(4)	92·2 (1)
Cl(2)–Cu–Cl(4)	156·0 (1)	Cl(3)–Cu–Cl(4)	94·6 (1)
C(2)–C(1)–N(6)	116·4 (4)	C(2)–C(1)–N(7)	125·1 (4)
N(6)–C(1)–N(7)	118·5 (5)	C(1)–C(2)–C(3)	119·6 (4)
C(1)–C(2)–Cl(8)	118·2 (4)	C(3)–C(2)–Cl(8)	122·2 (4)
C(2)–C(3)–C(4)	121·2 (5)	C(3)–C(4)–C(5)	119·4 (5)
C(3)–C(4)–Cl(9)	122·1 (4)	C(5)–C(4)–Cl(9)	118·5 (4)
C(4)–C(5)–N(6)	117·7 (4)	C(4)–C(5)–N(10)	125·8 (5)
N(6)–C(5)–N(10)	116·4 (4)	C(1)–N(6)–C(5)	125·6 (4)
C(12)–C(11)–N(16)	116·8 (4)	C(12)–C(11)–N(17)	126·4 (5)
N(16)–C(11)–N(17)	116·8 (5)	C(11)–C(12)–C(13)	120·0 (5)
C(11)–C(12)–Cl(18)	117·5 (4)	C(13)–C(12)–Cl(18)	122·4 (4)
C(12)–C(13)–C(14)	120·7 (5)	C(13)–C(14)–C(15)	120·4 (5)
C(13)–C(14)–Cl(19)	121·9 (4)	C(15)–C(14)–Cl(19)	117·7 (4)
C(14)–C(15)–N(16)	116·6 (4)	C(14)–C(15)–N(20)	126·4 (5)
N(16)–C(15)–N(20)	117·0 (5)	C(11)–N(16)–C(15)	125·1 (4)

(*c*) Hydrogen-bonding distances (Å)

N(6)–Cl(2)	3·077 (5)	H(6)–Cl(2)	2·179
N(7)–Cl(1)	3·310 (5)	H(7*A*)–Cl(1)	2·542
N(10)–Cl(3)	3·392 (5)	H(10*B*)–Cl(3)	2·466
N(10)–Cl(4)	3·265 (5)	H(10*A*)–Cl(4)	2·535
N(16)–Cl(1)	3·126 (5)	H(16)–Cl(1)	2·178
N(17)–Cl(4)	3·455 (5)	H(17*B*)–Cl(4)	2·496
N(20)–Cl(3)	3·351 (5)	H(20*A*)–Cl(3)	2·566

References

CAMPANA, C. F., SHEPHERD, D. F. & LITCHMAN, W. N. (1981). *Inorg. Chem.* **20**, 4039–4044.

DAVIES, G. & EL-SAYED, M. A. (1983). *Inorg. Chem.* **22**, 1257–1266.

FINKBEINER, H., HAY, A. S., BLANCHARD, H. S. & ENDRES, G. F. (1966). *J. Org. Chem.* **31**, 549–555.

GRIGEREIT, T., RAMAKRISHNA, B. L., PLACE, H., WILLETT, R. D., PELLACANI, G. C., MANFREDINI, T., MENABUE, L., BONAMARTINI-CORRADI, A. & BATTAGLIA, L. P. (1987). *Inorg. Chem.* **26**, 2235–2243.

HAY, A. S., BLANCHARD, H. S., ENDRES, G. F. & EUSTANCE, J. W. (1959). *J. Am. Chem. Soc.* **81**, 6335–6336.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JAMESON, R. F. & BLACKBURN, N. J. (1975). *J. Inorg. Nucl. Chem.* **37**, 809–814.

LOCKHART, T. P. (1983). *J. Am. Chem. Soc.* **105**, 1940–1946.

MARENGO-RULLÀN, J. & WILLETT, R. D. (1986). *Acta Cryst.* C**42**, 1487–1489.

NG, C. F. & LEUNG, K. S. (1981). *J. Catal.* **67**, 410–423.

PLACE, H. & WILLETT, R. D. (1987). *Acta Cryst.* C**43**, 1497–1500.

SHELDRICK, G. M. (1986). *SHELXTL Program Library*. Nicolet XRD Corporation, Madison, Wisconsin, USA.

SMITH, D. W. (1976). *Coord. Chem. Rev.* **21**, 93–144.

TAMURA, M. & KOCHI, J. K. (1971). *J. Chem. Soc. Jpn*, **44**, 3063–3073.
WILLETT, R. D. & BRENEMAN, G. L. (1983). *Inorg. Chem.* **22**, 326–329.
WILLETT, R. D. & GEISER, U. (1984). *Croat. Chem. Acta*, **57**, 737–747.
ZHELYAZKOVA, B. G. (1981). *Inorg. Nucl. Chem. Lett.* **17**, 141–145.

Acta Cryst. (1987). C**43**, 2303–2304

Structure of Bis(2-furaldehyde thiosemicarbazonato)nickel(II)*

BY VEDAVATI G. PURANIK, S. S. TAVALE AND T. N. GURU ROW†
Physical and Structural Chemistry Unit, National Chemical Laboratory, Pune 411008, *India*
AND P. UMAPATHY AND A. P. BUDHKAR
Inorganic Chemistry Division, National Chemical Laboratory, Pune 411008, *India*

(*Received* 11 *May* 1987; *accepted* 17 *July* 1987)

Abstract. $[Ni(C_6H_6N_3OS)_2]$, $M_r = 395{\cdot}1$, rhombohedral, $R\bar{3}$, $a = 10{\cdot}689\ (2)$ Å, $\alpha = 82{\cdot}04\ (2)°$, $V = 1188{\cdot}9\ (4)$ Å^3, $Z = 3$, $D_m = 1{\cdot}65\ (7)$, $D_x = 1{\cdot}655$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 1{\cdot}492$ mm^{-1}, $F(000) = 606$, $T = 293$ K, $R = 0{\cdot}028$ for 929 observed reflections. The Ni^{II} ion is in a distorted square-planar ligand field formed by the N_2S_2 chromophore. The planar furan rings are in a symmetric arrangement. The thiosemicarbazonato group is nearly planar.

Introduction. The α-(*N*)-heterocyclic carboxaldehyde thiosemicarbazones constitute a class of agents which possess both antineoplastic and antiviral activity. The correlation between antitumor activity and chelating ability of such compounds has been reported (Michaud & Sartorelli, 1968). Metal chelates of Pt^{II}, Pd^{II} and Ni^{II} with several ligands containing carboxaldehyde thiosemicarbazones have been synthesized in order to study the nature of the bonding and the stereochemistry. 2-Furaldehyde thiosemicarbazone has already been prepared (Sah & Daniels, 1950) and the title compound was prepared using this ligand.

Experimental. Crystals from alcohol, approximate dimensions $0{\cdot}15 \times 0{\cdot}25 \times 0{\cdot}4$ mm; D_m by flotation; Nonius CAD-4F-11M diffractometer; graphite-monochromated Mo $K\alpha$ radiation; $\omega/2\theta$ scan mode, scan speed 1° min^{-1}; $\theta < 23{\cdot}5°$, h 0 to 12, k −12 to 12, l −12 to 12. 3472 reflections collected, 929 judged significant ($|F_o| \geq 3\sigma|F_o|$). Lattice parameters from 25 reflections ($12 < 2\theta < 36°$); three standard reflections ($\bar{5}\bar{1}\bar{2}$, $\bar{4}0\bar{2}$ and $\bar{1}1\bar{5}$) every 1000 s, 3% variation in intensity. No correction for absorption. Structure was solved by direct methods, *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) using a modified procedure (Tavale & Guru Row, 1986). Full-matrix least-squares refinement (*LALS*; Gantzel, Sparks & Trueblood, 1961) of scale factor, positional and anisotropic thermal parameters (H atoms fixed geometrically, isotropic thermal parameters, not refined) converged to $R = 0{\cdot}028$ and $wR = 0{\cdot}028$; $\sum w(|F_o| - |F_c|)^2$ minimized, $w = (8{\cdot}5 + 1{\cdot}0|F_o| + 0{\cdot}014|F_o|^2)^{-1}$. Max. $(\Delta/\sigma) = 0{\cdot}1$. Final $\Delta\rho$ excursions $< |0{\cdot}2|$ e Å^{-3}. No correction for secondary extinction. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974).‡

Discussion. The atomic parameters with their e.s.d.'s and equivalent isotropic thermal parameters are given in Table 1. Bond lengths and bond angles involving non-H atoms are given in Table 2. Fig. 1 gives a perspective view of the molecule along with the numbering of atoms. Ni^{II} is in the distorted square-planar ligand field of the N_2S_2 chromophore as in [1,1′-(2,4-butanedione dihydrazono)-di-2,2′-phenylethanethiolato(2−)]nickel(II) (Hansen & Larsen, 1977), [2,5-hexanedione bis(4-phenylthiosemicarbazonato)]nickel(II) (Nandi, Chaudhuri, Mazumdar & Ghosh, 1984) and in bis(diiminosuccinonitrilo)nickel(II) (Peng, Wang & Chiang, 1984). The thiosemicarbazone group is planar with Ni—S = 2·149 (1) Å and Ni—N(2) = 1·921 (2) Å. The coordination around Ni is

* NCL Communication No. 4235.
† To whom all correspondence should be addressed.

‡ Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44264 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

0108-2701/87/122303-02$01.50