

Ni—N(2)	2.134 (3)	2.118 (3)
Ni—N(3)	2.085 (3)	2.089 (3)
Ni—N(4)	2.073 (3)	2.093 (2)
O(1)—Ni—O(3)	93.8 (1)	94.58 (9)
O(1)—Ni—N(1)	91.2 (1)	91.3 (1)
O(1)—Ni—N(2)	169.0 (1)	167.63 (9)
O(1)—Ni—N(3)	80.7 (1)	80.6 (1)
O(1)—Ni—N(4)	91.7 (1)	90.5 (1)
O(3)—Ni—N(1)	90.0 (1)	89.9 (1)
O(3)—Ni—N(2)	90.4 (1)	91.4 (1)
O(3)—Ni—N(3)	173.2 (1)	172.95 (9)
O(3)—Ni—N(4)	80.7 (1)	80.7 (1)
N(1)—Ni—N(2)	78.6 (1)	77.9 (1)
N(1)—Ni—N(3)	94.2 (1)	95.4 (1)
N(1)—Ni—N(4)	170.4 (1)	170.5 (1)
N(2)—Ni—N(3)	95.8 (1)	94.3 (1)
N(2)—Ni—N(4)	98.9 (1)	101.2 (1)
N(3)—Ni—N(4)	95.3 (1)	94.1 (1)

Table 3. Hydrogen-bonding geometry (Å, °)

D—H...A	D...A		D—H...A	
	(1)	(2)	(1)	(2)
O(W1)—H'(W1)...O(3)	2.789	2.765	178.8	177.0
O(W2)—H'(W2)...O(W1)	2.851	2.845	165.5	164.5
N(4')—H'(N4)...O(W2)	3.037	3.059	176.5	166.0
N(3 ^{iv})—H'(N3)...O(W2)	3.100	3.080	145.3	160.8
O(W2)—H'(W2)...O(W3)	2.861	2.869	158.7	141.7
O(W3)—H'(W3)...O(4 ⁱⁱⁱ)	2.814	2.804	160.0	167.3
O(W3)—H'(W3)...O(2 ^{iv})	2.677	2.707	153.8	169.3
N(4)—H'(N4)...O(2')	2.939	2.989	149.4	162.3
N(3)—H'(N3)...O(4 ⁱⁱⁱ)	3.088	3.017	163.4	159.0

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

E maps revealed all non-H atoms and the H atoms appeared on difference maps. Anisotropic displacement parameters were used for non-H atoms and isotropic displacement parameters for H atoms. Data reduction was carried out using the SDP software package (Enraf-Nonius, 1979). The structures were solved by direct methods using SHELXS86 (Sheldrick, 1985) and refined by least squares using SHELX76 (Sheldrick, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HR1020). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Addadi, L., Berkovitch-Yellin, Z., Weissbuch, I., Van Mil, J., Shimon, L. J. W., Lahav, M. & Leiserowitz, L. (1985). *Angew. Chem.* **24**, 466–485.
- Antolini, L., Battaglia, L. P., Bonamartini Corradi, A., Marcotrigiano, G., Menabue, L., Pellacani, G. C., Saladini, M. & Sola, M. (1986). *Inorg. Chem.* **25**, 2901–2904.
- Antolini, L., Marcotrigiano, G., Menabue, L. & Pellacani, G. C. (1983). *Inorg. Chem.* **22**, 141–145.
- Antolini, L., Marcotrigiano, G., Menabue, L., Pellacani, G. C., Saladini, M. & Sola, M. (1985). *Inorg. Chem.* **24**, 3621–3626.
- Brezina, F., Sindelar, Z., Kameníček, J. & Lasovsky, J. (1988). *Collect. Czech Chem. Commun.* **53**, 563–570.
- Desiraju, G. R. (1989). *Crystal Engineering. The Design of Organic Solids*, p. 85. Amsterdam: Elsevier.
- Enraf-Nonius (1979). *Structure Determination Package*. Enraf-Nonius, Delft, The Netherlands.
- Freeman, H. C. & Guss, J. M. (1968). *Acta Cryst.* **B24**, 1133–1135.
- Freeman, H. C. & Guss, J. M. (1978). *Acta Cryst.* **B34**, 2451–2458.
- Johnson, C. K. (1965). ORTEP. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

- Poletti, D., Stojaković, D. R., Prelesnik, B. V. & Manojlović-Muir, Lj. (1990). *Acta Cryst.* **C46**, 399–402.
- Sheldrick, G. M. (1976). SHELX76. Program for Crystal Structure Determination. Univ. of Cambridge, England.
- Sheldrick, G. M. (1985). SHELXS86. Program for the Solution of Crystal Structures. Univ. of Göttingen, Germany.
- Skoulika, S., Michaelides, A. & Aubry, A. (1991). *J. Cryst. Growth*, **108**, 285–289.
- Žák, Z., Głowiak, T., Kameníček, J. R. & Březina, F. (1990). *Acta Cryst.* **C46**, 2073–2075.

Acta Cryst. (1995). **C51**, 846–849

[3,9-Dimethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioximato(1-)](thiocyanato)-copper(II) and [3,6,6,9-Tetramethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioximato(1-)](isothiocyanato)copper(II)

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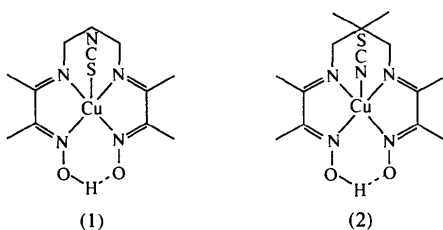
Abstract

The coordination geometries about the Cu^{II} ions in both [3,9-dimethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioximato(1-)](thiocyanato)copper(II), [Cu(C₁₁H₁₉N₄O₂)(SCN)] (1), and [3,6,6,9-tetramethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioximato(1-)](isothiocyanato)copper(II), [Cu(C₁₃H₂₃N₄O₂)(NCS)] (2), are distorted square pyramidal with the four diazadioxime N atoms in equatorial positions and the monodentate ligand axial. This monodentate axial ligand is an S-bonded thiocyanato group in complex (1) and an N-bonded isothiocyanato group in (2). The intramolecular O...O hydrogen-bond lengths are 2.530 (4) and 2.490 (2) Å in complexes (1) and (2), respectively.

Comment

Metal–thiocyanato complexes have been investigated extensively in order to solve the interesting problem

of whether the thiocyanato group is bonded to the metal through the N atom ($M-NCS$), through the S atom ($M-SCN$) or through both by means of bridging ($M-NCS-M$) (Mitchell & Williams, 1960). It has been suggested by Pearson (1963) that the S atom in SCN^- is soft and prefers to coordinate with soft acids (class *b* metals), whereas N in SCN^- is hard and coordinates with hard acids (class *a* metals) (Ahrlund, Chatt & Davies, 1958). However, other factors, such as the oxidation state of the metal, the nature of other ligands in the complex and steric effects, also influence the mode of coordination (Bennett, Clark & Goodwin, 1967). We have reported previously the structure of [3,10-dimethyl-4,9-diaza-3,9-dodecadiene-2,11-dione dioximato(1-)](isothiocyanato)copper(II), $[Cu(C_{12}H_{21}N_4O_2)(NCS)]$ (3) (Tahirov, Lu, Luh & Chung, 1993). This paper is concerned with the coordination of the ambidentate thiocyanate ligand in two diazadioxime copper(II) complexes, (1) and (2).



The coordination geometries about the Cu^{II} ions of both complexes are distorted square pyramidal with the four N atoms of the tetradentate ligand in equatorial positions and the monodentate ligand axial. This monodentate axial ligand is an S-bonded thiocyanato group in complex (1) and an N-bonded isothiocyanato group in (2). The steric requirements of the ambidentate ligand play an important role in the structures of these complexes. The two C(6) methyl groups of 3,6,6,9-tetramethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioxime [(DOH)₂-6,6-Me₂-Pn] hinder the formation of the S-bonded complex; therefore, in complex (2), the isothiocyanato group is N-bonded. The equatorial N atoms of both complexes undergo slight tetrahedral distortion. The maximum deviation of the four equatorial N atoms from the least-squares plane formed by the four equatorial N atoms is 0.012(5) Å in complex (1) and 0.034(2) Å in (2). In complex (1), the deviation of the Cu^{II} ion from the equatorial least-squares plane is 0.336(2) Å in the direction of the thiocyanato S atom. In complex (2), this deviation is 0.351(1) Å towards the isothiocyanato N atom. The equatorial Cu—N distances of complexes (1) and (2) are very similar, indicating that the electronic effects of these two tetradentate ligands are about the same. In complex (3), however, the average Cu—N distance is slightly longer due to a tetrahedral distortion of the equatorial N atoms. In complex (1), the ambiden-

tate thiocyanate ligand is bonded through the S atom with an axial Cu—S—C angle of 98.8(2)°, whereas in both (2) and (3) this ligand is almost parallel to the axial Cu—N bond with Cu—N—C angles of 175.9(2) and 172.8(5)°, respectively. Complexes (1) and (2) differ in that (2) has two methyl groups on atom C(6) and the six-membered chelate ring has a chair conformation, whereas the equivalent ring in (1) has a boat conformation. Because the conformation of the six-membered ring changes from boat in (1) to chair in (2) on addition of two methyl groups, these two methyl groups are moved away from the NCS^- ligand.

An oxime proton is lost from the diazadioxime ligand in the formation of the complex and the remaining

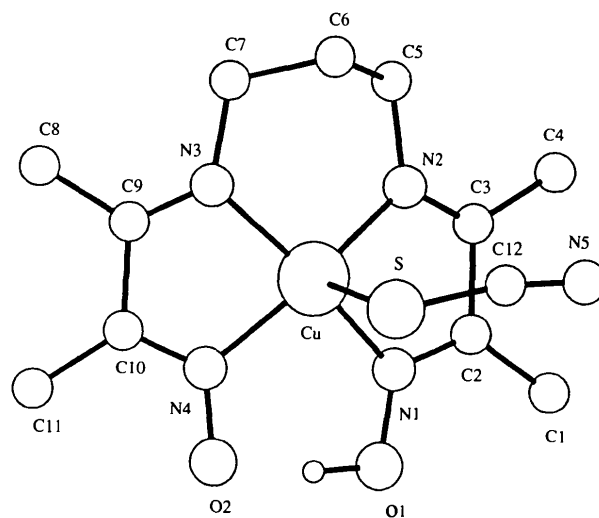


Fig. 1. A perspective view of complex (1) with H atoms excluded for clarity.

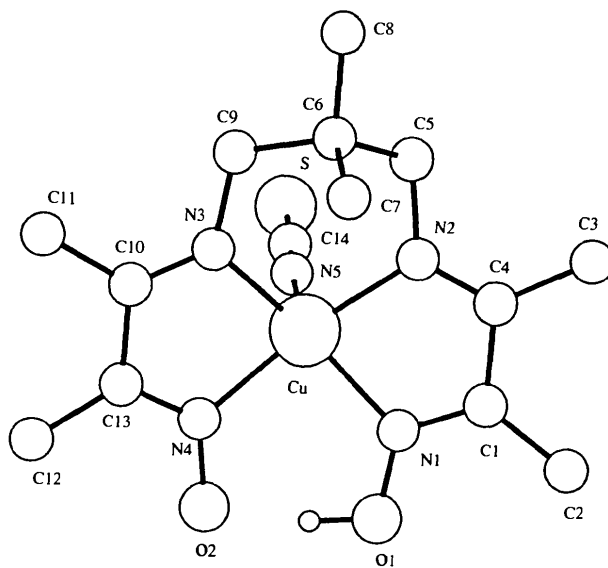


Fig. 2. A perspective view of complex (2) with H atoms excluded for clarity.

oxime proton forms a strong intramolecular hydrogen bond. The O...O distances are 2.530 (4), 2.490 (2) and 2.461 (6) Å for complexes (1), (2) and (3), respectively, the S-bonded thiocyanato complex having a longer O...O distance than that of the N-bonded isothiocyanato complex.

Experimental

The 3,9-dimethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioxime ligand [(DOH)₂Pn] was prepared using the method of Wang, Chung & Cheng (1990). The diazadioxime complex was prepared by the following procedure. CuSO₄·5H₂O (6 mmol) and (DOH)₂Pn (7 mmol) were dissolved in water (20 ml). Sufficient NaOH solution (0.1 M) was added to neutralize this acidic solution. The resulting solution was heated on a steam-bath for ca 1 h and then cooled to room temperature. Excess NaSCN was added and the solution was left to stand for ca 1 h after which time black crystals of (1) were deposited. Single crystals suitable for X-ray structure determination were obtained from methanol solution. The 3,6,6,9-tetramethyl-4,8-diaza-3,8-undecadiene-2,10-dione dioxime ligand [(DOH)₂-6,6-Me₂-Pn] was prepared using the method of Lu, Tseng, Luh & Chung (1993). Complex (2) was prepared by the same procedure as for (1). Deep violet crystals suitable for X-ray structure determination were obtained from methanol solution.

Compound (1)

Crystal data

[Cu(C₁₁H₁₉N₄O₂)(SCN)]

M_r = 360.92

Triclinic

*P*1̄

a = 7.275 (3) Å

b = 7.7110 (7) Å

c = 14.293 (1) Å

α = 90.152 (7)°

β = 98.77 (1)°

γ = 100.49 (2)°

V = 778.9 (4) Å³

Z = 2

D_x = 1.539 Mg m⁻³

Data collection

Enraf-Nonius CAD-4 diffractometer

θ/2θ scans

Absorption correction:

ψ scan (North, Phillips & Mathews, 1968)

T_{min} = 0.786, *T_{max}* = 0.999

7252 measured reflections

6839 independent reflections

Refinement

Refinement on *F*

R = 0.064

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 8.05–21.53°

μ = 1.54 mm⁻¹

T = 298 (3) K

Parallelepiped

0.45 × 0.28 × 0.28 mm

Black

4193 observed reflections

[*I* > 2.5σ(*I*)]

R_{int} = 0.042

θ_{max} = 35°

h = -11 → 11

k = 0 → 12

l = -22 → 23

3 standard reflections

frequency: 60 min

intensity decay: 1.5%

Δρ_{max} = 1.32 (18) e Å⁻³

Δρ_{min} = -1.12 (18) e Å⁻³

wR = 0.099

S = 2.37

4193 reflections

191 parameters

H-atom parameters not refined

w = 1/[σ²(*F*) + 0.0008*F*²]

(Δ/σ)_{max} = 0.001

Compound (2)

Crystal data

[Cu(C₁₃H₂₃N₄O₂)(NCS)]

M_r = 388.97

Monoclinic

*P*2₁/n

a = 8.099 (2) Å

b = 10.638 (2) Å

c = 19.870 (2) Å

β = 92.70 (2)°

V = 1710.0 (5) Å³

Z = 4

D_x = 1.511 Mg m⁻³

Data collection

Enraf-Nonius CAD-4 diffractometer

θ/2θ scans

Absorption correction:

ψ scan (North, Phillips & Mathews, 1968)

T_{min} = 0.918, *T_{max}* = 0.999

5414 measured reflections

4966 independent reflections

Refinement

Refinement on *F*

R = 0.031

wR = 0.050

S = 1.30

4073 reflections

209 parameters

H-atom parameters not refined

w = 1/[σ²(*F*) + 0.001*F*²]

(Δ/σ)_{max} = 0.004

Extinction correction:

Zachariasen (1967)

Extinction coefficient: 0.7 (1)

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 8.20–17.60°

μ = 1.41 mm⁻¹

T = 298 (3) K

Parallelepiped

0.46 × 0.31 × 0.25 mm

Deep violet

4073 observed reflections

[*I* > 2.5σ(*I*)]

R_{int} = 0.020

θ_{max} = 29.9°

h = -11 → 11

k = 0 → 14

l = 0 → 27

3 standard reflections

frequency: 60 min

intensity decay: 1.0%

Δρ_{max} = 0.49 (7) e Å⁻³

Δρ_{min} = -0.53 (7) e Å⁻³

Extinction correction:

Zachariasen (1967)

Extinction coefficient:

1.04 (9)

Atomic scattering factors

from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

Compound (1)	$B_{eq} = (8\pi^2/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$			<i>B_{eq}</i>
	<i>x</i>	<i>y</i>	<i>z</i>	
Cu	0.09269 (6)	0.38415 (6)	0.31118 (3)	2.782 (18)
S	0.3526 (2)	0.2739 (2)	0.24394 (11)	5.39 (6)
O1	-0.1156 (5)	0.0200 (4)	0.3228 (2)	3.74 (12)
O2	0.0984 (5)	0.1546 (4)	0.4713 (2)	3.74 (12)
N1	-0.1005 (5)	0.1709 (4)	0.2730 (2)	3.05 (11)
N2	-0.0426 (5)	0.4676 (5)	0.1954 (3)	3.31 (12)
N3	0.2160 (5)	0.6172 (4)	0.3682 (3)	3.17 (12)
N4	0.1474 (5)	0.3183 (4)	0.4432 (2)	3.02 (12)
N5	0.1756 (6)	0.1752 (6)	0.0643 (2)	4.12 (17)
C1	-0.3309 (7)	0.0146 (8)	0.1432 (4)	4.8 (2)
C2	-0.1995 (5)	0.1708 (6)	0.1902 (3)	3.31 (15)

C3	-0.1674 (6)	0.3489 (7)	0.1475 (3)	3.77 (17)	O1—N1	1.343 (2)	C6—C7	1.524 (3)
C4	-0.2872 (8)	0.3726 (11)	0.0548 (4)	6.6 (3)	O2—N4	1.335 (2)	C6—C8	1.538 (2)
C5	0.0032 (7)	0.6530 (7)	0.1684 (4)	4.9 (2)	N1—C1	1.292 (2)	C6—C9	1.550 (2)
C6	0.2040 (8)	0.7374 (7)	0.2081 (4)	4.6 (2)	N2—C4	1.283 (2)	C10—C11	1.501 (2)
C7	0.2464 (8)	0.7787 (6)	0.3131 (4)	4.4 (2)	N2—C5	1.459 (2)	C10—C13	1.487 (2)
C8	0.3595 (7)	0.7786 (6)	0.5170 (4)	4.2 (2)	N3—C9	1.467 (2)	C12—C13	1.492 (2)
C9	0.2688 (5)	0.6180 (5)	0.4581 (3)	3.09 (14)	N3—C10	1.286 (2)		
C10	0.2298 (5)	0.4441 (5)	0.5034 (3)	2.86 (13)	N1—Cu—N2	80.20 (6)	C4—N2—C5	124.5 (1)
C11	0.2797 (7)	0.4160 (7)	0.6067 (3)	3.90 (17)	N1—Cu—N3	157.63 (6)	Cu—N3—C9	121.7 (1)
C12	0.2471 (7)	0.2319 (7)	0.1364 (5)	5.3 (3)	N1—Cu—N4	94.00 (6)	Cu—N3—C10	113.7 (1)
Compound (2)					N1—Cu—N5	104.00 (6)	C9—N3—C10	123.7 (1)
Cu	0.61591 (2)	0.87961 (2)	0.14671 (1)	2.063 (8)	N2—Cu—N3	97.85 (6)	Cu—N4—O2	123.3 (1)
S	0.37177 (7)	0.88292 (6)	0.36662 (3)	3.99 (2)	N2—Cu—N4	161.13 (6)	Cu—N4—C13	115.9 (1)
O1	0.79849 (18)	1.11794 (10)	0.15233 (8)	3.27 (5)	N2—Cu—N5	96.60 (6)	O2—N4—C13	120.7 (1)
O2	0.51636 (19)	1.12766 (11)	0.09705 (8)	3.58 (6)	Cu—N5—C14	175.9 (2)	N2—C5—C6	112.9 (1)
N1	0.80650 (17)	0.99311 (12)	0.16207 (7)	2.38 (5)	N1—C1—C2	123.7 (2)	C5—C6—C7	110.0 (1)
N2	0.78924 (16)	0.75531 (12)	0.17075 (7)	2.16 (4)	N1—C1—C4	112.3 (1)	C5—C6—C8	106.4 (1)
N3	0.46134 (16)	0.76534 (13)	0.09635 (7)	2.30 (5)	C2—C1—C4	124.0 (1)	C5—C6—C9	113.5 (1)
N4	0.48344 (18)	1.00472 (13)	0.09561 (7)	2.50 (5)	N2—C4—C1	115.4 (1)	C7—C6—C8	110.2 (1)
N5	0.50269 (19)	0.87737 (15)	0.23965 (8)	3.21 (7)	N2—C4—C3	125.7 (2)	C7—C6—C9	110.8 (2)
C1	0.94288 (19)	0.94203 (15)	0.18458 (8)	2.28 (5)	C1—C4—C3	119.0 (1)	C8—C6—C9	105.7 (1)
C2	1.0970 (2)	1.01452 (18)	0.20204 (11)	3.24 (7)	N3—Cu—N4	80.66 (6)	N3—C9—C6	113.7 (1)
C3	1.0710 (2)	0.73045 (18)	0.22204 (11)	3.51 (8)	N3—Cu—N5	98.36 (6)	N3—C10—C11	125.4 (2)
C4	0.92853 (19)	0.80229 (15)	0.19140 (8)	2.21 (5)	N4—Cu—N5	102.24 (6)	N3—C10—C13	115.9 (1)
C5	0.7470 (2)	0.62224 (14)	0.17450 (9)	2.58 (6)	Cu—N1—O1	123.4 (1)	C11—C10—C13	118.0 (2)
C6	0.6464 (2)	0.57531 (14)	0.11163 (8)	2.31 (5)	Cu—N1—C1	116.5 (1)	N4—C13—C10	112.9 (1)
C7	0.7388 (3)	0.60392 (18)	0.04837 (10)	3.29 (7)	O1—N1—C1	120.0 (1)	N4—C13—C12	122.7 (2)
C8	0.6270 (2)	0.43246 (16)	0.12025 (11)	3.18 (7)	Cu—N2—C4	114.9 (1)	C10—C13—C12	124.5 (2)
C9	0.4683 (2)	0.62859 (15)	0.10563 (10)	2.79 (6)	Cu—N2—C5	119.8 (1)	S—C14—N5	178.3 (2)
C10	0.3423 (2)	0.82254 (16)	0.06410 (8)	2.38 (5)				
C11	0.1937 (2)	0.7602 (2)	0.03060 (11)	3.68 (8)				
C12	0.2329 (3)	1.0456 (2)	0.02528 (10)	3.66 (7)				
C13	0.3546 (2)	0.96192 (16)	0.06189 (8)	2.47 (5)				
C14	0.4493 (2)	0.87798 (14)	0.29267 (9)	2.51 (6)				

Table 2. Selected geometric parameters (Å, °)

Compound (1)			
Cu—S	2.521 (2)	N3—C9	1.284 (6)
Cu—N1	1.974 (3)	N4—C10	1.292 (5)
Cu—N2	1.965 (3)	N5—C12	1.129 (8)
Cu—N3	1.970 (3)	C1—C2	1.482 (7)
Cu—N4	1.956 (3)	C2—C3	1.499 (7)
S—C12	1.613 (7)	C3—C4	1.502 (6)
O1—N1	1.362 (4)	C5—C6	1.509 (8)
O2—N4	1.329 (4)	C6—C7	1.507 (8)
N1—C2	1.288 (5)	C8—C9	1.485 (6)
N2—C3	1.278 (6)	C9—C10	1.490 (5)
N2—C5	1.474 (6)	C10—C11	1.491 (6)
N3—C7	1.476 (5)		
S—Cu—N1	95.1 (1)	Cu—N4—O2	122.6 (2)
S—Cu—N2	100.0 (1)	Cu—N4—C10	116.5 (3)
S—Cu—N3	103.9 (1)	O2—N4—C10	120.8 (3)
S—Cu—N4	100.2 (1)	N1—C2—C1	124.4 (4)
N1—Cu—N2	80.3 (1)	N1—C2—C3	111.7 (4)
N1—Cu—N3	161.0 (1)	C1—C2—C3	124.0 (4)
N1—Cu—N4	94.8 (1)	N2—C3—C2	116.1 (4)
N2—Cu—N3	97.5 (2)	N2—C3—C4	126.4 (5)
N2—Cu—N4	159.5 (1)	C2—C3—C4	117.5 (5)
N3—Cu—N4	80.8 (1)	N2—C5—C6	112.0 (4)
Cu—S—C12	98.8 (2)	C5—C6—C7	116.8 (5)
Cu—N1—O1	123.8 (2)	N3—C7—C6	111.5 (4)
Cu—N1—C2	116.3 (3)	N3—C9—C8	124.2 (4)
O1—N1—C2	119.3 (3)	N3—C9—C10	115.8 (3)
Cu—N2—C3	114.6 (3)	C8—C9—C10	120.0 (4)
Cu—N2—C5	120.7 (3)	N4—C10—C9	112.5 (3)
C3—N2—C5	124.7 (4)	N4—C10—C11	123.1 (4)
Cu—N3—C7	123.4 (3)	C9—C10—C11	124.4 (4)
Cu—N3—C9	114.4 (3)	S—C12—N5	168.9 (5)
C7—N3—C9	122.1 (4)		
Compound (2)			
Cu—N1	1.972 (1)	N4—C13	1.296 (2)
Cu—N2	1.971 (1)	N5—C14	1.157 (3)
Cu—N3	1.982 (1)	C1—C2	1.494 (2)
Cu—N4	1.962 (1)	C1—C4	1.498 (2)
Cu—N5	2.100 (2)	C3—C4	1.490 (2)
S—C14	1.626 (2)	C5—C6	1.542 (2)

Both structures were solved by direct and Fourier methods and refined by full-matrix least squares. H atoms were located by the difference Fourier method. The data were reduced and the structures solved and refined using NRCVAX (Gabe, Le Page, White & Lee, 1987).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

- Ahrland, S., Chatt, J. & Davies, N. R. (1958). *Q. Rev. Chem. Soc.* **12**, 265–269.
- Bennett, M. A., Clark, R. J. H. & Goodwin, A. D. J. (1967). *Inorg. Chem.* **6**, 1625–1631.
- Gabe, E. J., Le Page, Y., White, P. S. & Lee, F. L. (1987). *Acta Cryst.* **A43**, C-294.
- Lu, T. H., Tseng, F., Luh, H. & Chung, C. S. (1993). *Acta Cryst.* **C49**, 666–668.
- Mitchell, P. C. H. & Williams, R. J. P. (1960). *J. Chem. Soc.* pp. 1912–1918.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Pearson, R. G. (1963). *J. Am. Chem. Soc.* **85**, 3533–3539.
- Tahirov, T., Lu, T. H., Luh, H. & Chung, C. S. (1993). *Acta Cryst.* **C49**, 801–803.
- Wang, Y. M., Chung, C. S. & Cheng, C. Y. (1990). *Acta Cryst.* **C46**, 1429–1432.
- Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.