O(5)—Cd(1)—O(2)	103.90 (11)	O(1)—C(1)—C(2)	118.4 (4)
O(2^{i})—Cd(1)—O(2)	172.77 (14)	C(3)—C(2)—C(1)	111.3 (3)
O(2W^{ii})—Cd(2)—O(2W)	77.8 (2)	C(3)—C(2)—N(1)	112.0 (3)
O(2W^{ii})—Cd(2)—O(3)	93.28 (12)	C(1)—C(2)—N(1)	110.2 (3)
O(2W)—Cd(2)—O(3)	95.18 (13)	C(2)—C(3)—C(4)	110.5 (3)
O(3)—Cd(2)—O(3^{ii})	169.1 (2)	C(5)—C(4)—C(3)	110.3 (3)
O(2W^{ii})—Cd(2)—O(4)	143.77 (11)	C(4)—C(5)—N(2)	111.9 (3)
O(2W)—Cd(2)—O(4)	114.76 (11)	C(4)—C(5)—C(6)	110.6 (3)
O(3)—Cd(2)—O(4)	53.32 (11)	N(2)—C(5)—C(6)	111.5 (3)
O(3)—Cd(2)—O(4^{ii})	116.62 (12)	O(3)—C(6)—O(4)	122.6 (4)
O(4)—Cd(2)—O(4^{ii})	76.1 (2)	O(3)—C(6)—C(5)	116.8 (4)
C(1)—O(1)—Cd(1)	94.9 (2)	O(4)—C(6)—C(5)	120.5 (4)
C(1)—O(2)—Cd(1)	88.3 (3)	O(6)—N(3)—O(7)	119.7 (5)
C(6)—O(3)—Cd(2)	97.0 (3)	O(6)—N(3)—O(5)	118.6 (5)
C(6)—O(4)—Cd(2)	86.9 (3)	O(7)—N(3)—O(5)	121.6 (5)
C(7)—N(1)—C(8)	108.8 (3)	N(3)—O(5)—Cd(1)	113.4 (3)
C(7)—N(1)—C(9)	107.2 (3)	O(10)—N(4)—O(9)	122.2 (4)
C(8)—N(1)—C(9)	109.1 (3)	O(10)—N(4)—O(8)	119.7 (4)
C(7)—N(1)—C(2)	109.3 (3)	O(9)—N(4)—O(8)	118.1 (4)

$X\cdots Y\cdots Z$	$X\cdots Y$	$Y\cdots Z$	$X\cdots Y\cdots Z$
O(1)···O(1W^{iii})···O(1^{i})	2.683 (5)	–	72.4 (2)
O(8)···O(2W)···O(4^{iii})	2.744 (5)	2.771 (5)	113.4 (2)

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

The structure was solved with the Patterson superposition method. H atoms of the double-betaine molecule were generated geometrically (C—H = 0.96 Å) and the aqua H atoms were located in difference Fourier maps. All H atoms were assigned isotropic displacement parameters and included in the structure-factor calculations. All computations were performed on a PC 486 computer.

Data collection: *P3/PC Diffractometer Control Program* (Siemens, 1989). Cell refinement: *P3/PC Diffractometer Control Program*. Data reduction: *SHELXTL-Plus XDISK* (Sheldrick, 1987). Program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *SHELXTL/PC XP*. Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: JZ1080). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Isothiocyanatobis(1,10-phenanthroline)copper(II) Tricyanomethanide

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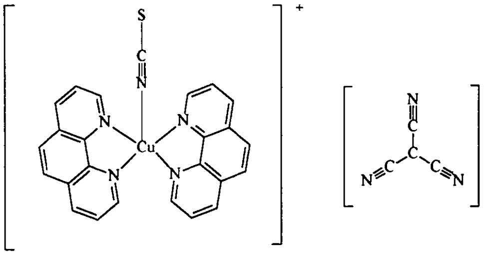
Abstract

The crystal structure of $[Cu(NCS)(C_{12}H_8N_2)_2][C(CN)_3]$ is presented here. The structure comprises discrete $[Cu(phen)_2(NCS)]^+$ cations and $[C(CN)_3]^-$ anions. The coordination polyhedron of Cu^{II} is a distorted trigonal bipyramid with a CuN_5 chromophore.

Comment

The title compound, $[Cu(phen)_2(NCS)][C(CN)_3]$, (I), where phen = 1,10-phenanthroline, was prepared and its crystal structure solved as part of our study concerning changes in the shape of the $[Cu(phen)_2X]^+$ cation [X^- = pseudohalide anion (1−)] resulting from alteration of the out-of-sphere anion.



(I)

Recently, we have published the structure of $[Cu(phen)_2(NCS)][(ON)C(CN)_2]$, (II), with $NCS^- = X^-$ and $(ON)C(CN)_2^-$ (dicyanonitrosomethanide) as the out-of-sphere anion (Potočňák, Dunaj-Jurčo, Mikloš, Kabešová & Jäger, 1995). We decided to prepare a compound with a $[\mathrm{Cu(phen)_2(NCS)}]^+$ cation and the similar anion $\mathrm{C(CN)_3^-}$ (tcm$^-$) to evaluate changes in the $\mathrm{Cu^{II}}$ coordination polyhedron caused by changing the out-of-sphere anion. The crystal structure comprises discrete $[\mathrm{Cu(phen)_2(NCS)}]^+$ cations and $\mathrm{C(CN)_3^-}$ anions.

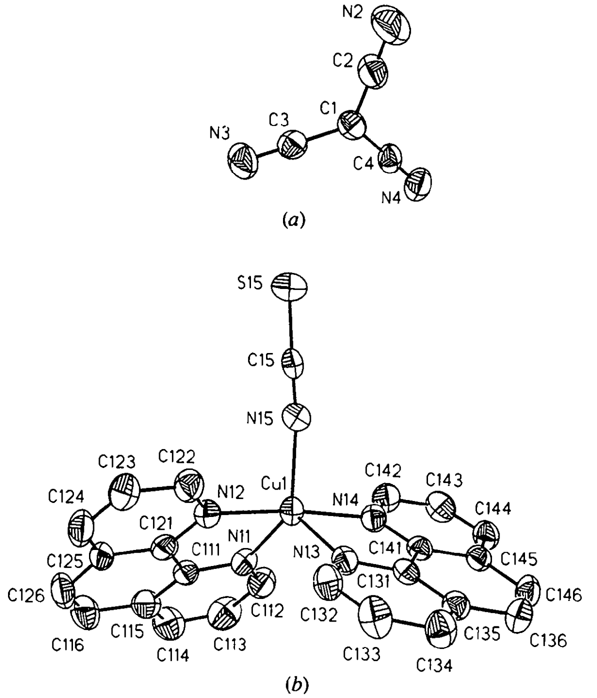


Fig. 1. *ORTEP* (Johnson, 1965) drawings of (*a*) the anion and (*b*) the cation of the formula unit, with labelling of the atoms. Displacement ellipsoids are plotted at the 40% probability level.

Fig. 1 shows the labelling scheme of one formula unit. The $\mathrm{Cu^{II}}$ atom is fivefold coordinated by two phen molecules and by one $\mathrm{NCS^-}$ ligand (in the equatorial plane) through the N atoms. The coordination polyhedron is a distorted trigonal bipyramid. The tcm$^-$ anion does not enter the inner coordination sphere. In the trigonal bipyramid, the two out-of-plane Cu1—N12 and Cu1—N14 distances have similar values [1.987 (3) and 2.000 (3) Å, respectively], and are almost linear [N12—Cu1—N14 = 173.95 (12)°]. The two in-plane distances (Cu1—N11 and Cu1—N13) also have similar values [2.078 (3) and 2.112 (3) Å, respectively], but they are longer on average than the out-of-plane Cu—N distances by 0.101 Å. All these values agree very well with those for the $\mathrm{(ON)C(CN)_2^-}$ compound, (II): the out-of-plane distances are on average 1.987 (7) Å and make an angle of 172.24 (11)° and the two in-plane distances average 2.092 (10) Å. The third in-plane Cu1—N15 distance of 1.984 (4) Å is significantly shorter than the other two; for (II), this distance is even shorter [1.963 (3) Å]. In a recently published paper (Parker, Manson & Breneman, 1994) describing the structure of $[\mathrm{Cu(phen)_2(NCS)}]\mathrm{ClO_4}$, (III), the corresponding out-of-plane and in-plane distances are somewhat longer [average 2.002 (4) Å] and somewhat shorter [average 2.069 (4) Å], respectively, but the Cu—N(NCS) distance is substantially longer [2.005 (4) Å] than those in the two structures (I) and (II). The out-of-plane angles for the title compound are within 80.5 (1)–96.6 (1)° [80.5 (1)–95.9 (1) and 80.4 (2)–97.6 (1)° for (II) and (III), respectively].

Two bond angles in the equatorial plane differ considerably from the ideal trigonal angle of 120°, with one large angle of 126.62 (14)° (α_1 = N15—Cu1—N11) and one small angle of 113.19 (13)° (α_2 = N15—Cu1—N13). The third angle (α_3 = N11—Cu1—N13 = 120.16 (12)°) has an almost ideal trigonal value. Thus, relative to a regular trigonal bipyramidal $\mathrm{CuN_5}$ chromophore, the Cu1—N15 bond which is opposite the angle α_3 shows a shortening and there is a difference of 13.43° between α_1 and α_2 [for (II), α_1, α_2 and α_3 are 127.96 (12), 115.81 (12) and 116.21 (10)°, respectively; for (III) they are 125.9 (2), 118.0 (2) and 116.1 (1)°, respectively].

According to Harrison & Hathaway (1980), the coordination polyhedron around the Cu atom can be best described as trigonal bipyramidal with near C_{2v} symmetry. The sum of the bond angles in the equatorial plane (359.97°) indicates coplanarity of the Cu atom with the three coordinating atoms N11, N13 and N15 [deviation of Cu1 from the plane of N11, N13 and N15 is 0.017 (2) Å].

For steric reasons, in the trigonal-bipyramidal polyhedron the N atoms of the two phen molecules are coordinated both in equatorial and axial positions. The bond distances and angles in the phen molecules are quite normal and range from 1.337 (7) to 1.445 (5) Å and 116.5 (4) to 124.6 (4)°, respectively. Both phen molecules are nearly planar; the largest deviation of atoms from the mean planes is less than 0.036 (5) Å. The mean planes of the two phen molecules are inclined at 119.04 (7)°.

The thiocyanato ligand is bound to the Cu atom through the N atom. The anion is linear [N15—C15—S15 = 178.2 (4)°], with N15—C15 and C15—S15 bond distances of 1.137 (5) and 1.612 (4) Å, respectively. The coordination of the $\mathrm{NCS^-}$ anion to the $\mathrm{Cu^{II}}$ atom involves a significant deviation of the Cu1—N15—C15 angle [172.5 (3)°] from linearity. This angle in compound (II) is 166.1 (5)°; the values for compounds (II) and (III) are close to those found in (I).

The almost planar tcm$^-$ anion [the largest deviation of atoms from the mean plane is less than 0.025 (7) Å] is uncoordinated, probably due to steric repulsion, and serves as a counterion to the $[\mathrm{Cu(phen)_2(NCS)}]^+$ cation. The mode of bonding in this anion can be described as a largely delocalized π-bonding system (Golub, Köhler & Skopenko, 1986). According to this assumption the C1—Cn ($n = 2,3,4$) bonds [1.387(6), 1.400(6) and

1.395 (6) Å, respectively] are considerably shorter than single C_{sp^2}—C_{sp} bonds (1.440 Å). But, contrary to this assumption, the $Cn{\equiv}Nn$ ($n = 2,3,4$) bond lengths [1.147 (6), 1.143 (5) and 1.145 (6) Å, respectively] are slightly shorter than normal C≡N triple-bond lengths (1.153 Å). The values of the angles around the central C1 atom are close to the ideal value of 120°, while the $C1{-}Cn{\equiv}Nn$ ($n = 2,3,4$) angles are almost linear.

Experimental

Crystals were prepared by mixing 10 ml of a 0.1 *M* aqueous solution of $Cu(NO_3)_2$ with 20 ml of a 0.1 *M* ethanol solution of phen. A mixture of 10 ml of a 0.1 *M* ethanol solution of $KC(CN)_3$ and 10 ml of a 0.1 *M* water solution of KSCN was added. The light-green precipitate which appeared after several minutes was dissolved by adding 60 ml of NH_4OH and 25 ml of ethanol. After several days dark green prismatic crystals of (I) appeared. The density D_m was measured by flotation in benzene/bromoform.

Crystal data

$[Cu(NCS)(C_{12}H_8N_2)_2][C(CN)_3]$
$M_r = 572.10$
Triclinic
$P\overline{1}$
$a = 7.930 (4)$ Å
$b = 11.018 (4)$ Å
$c = 15.512 (6)$ Å
$\alpha = 96.01 (3)°$
$\beta = 98.93 (3)°$
$\gamma = 108.00 (3)°$
$V = 1256.4 (9)$ Å^3
$Z = 2$
$D_x = 1.512$ Mg m^{-3}
$D_m = 1.49$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 4.75–12.64°$
$\mu = 0.989$ mm^{-1}
$T = 292 (2)$ K
Prism
0.4 × 0.35 × 0.15 mm
Dark green

Data collection

Syntex $P2_1$ diffractometer
θ–2θ scans
Absorption correction: none
4435 measured reflections
4435 independent reflections
3221 observed reflections [$I > 2\sigma(I)$]

$\theta_{max} = 25.00°$
$h = 0 \rightarrow 10$
$k = -14 \rightarrow 13$
$l = -20 \rightarrow 19$
2 standard reflections monitored every 98 reflections intensity decay: 4%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0460$
$wR(F^2) = 0.1198$
$S = 1.004$
4384 reflections
416 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0930P)^2 + 0.5345P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.454$ e Å^{-3}
$\Delta\rho_{min} = -0.489$ 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)*

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

	x	y	z	U_{eq}
Cu1	0.37225 (6)	0.40224 (4)	0.22620 (3)	0.0447 (2)
N11	0.3382 (4)	0.2639 (3)	0.3092 (2)	0.0452 (7)
N12	0.5685 (4)	0.5006 (3)	0.3286 (2)	0.0453 (7)
N13	0.5421 (4)	0.4060 (3)	0.1335 (2)	0.0417 (7)
N14	0.1894 (4)	0.2904 (3)	0.1216 (2)	0.0440 (7)
N15	0.2639 (5)	0.5422 (4)	0.2249 (2)	0.0570 (9)
C15	0.2149 (5)	0.6286 (4)	0.2326 (2)	0.0449 (9)
S15	0.1449 (2)	0.75126 (13)	0.24019 (9)	0.0834 (4)
C1	0.3255 (6)	0.8919 (4)	0.7385 (3)	0.0524 (10)
C2	0.3015 (6)	0.9915 (5)	0.6957 (3)	0.0676 (12)
N2	0.2788 (8)	1.0732 (5)	0.6603 (4)	0.114 (2)
C3	0.4591 (6)	0.9162 (4)	0.8147 (3)	0.0563 (10)
N3	0.5655 (6)	0.9343 (4)	0.8776 (3)	0.0818 (13)
C4	0.2118 (5)	0.7654 (4)	0.7058 (2)	0.0510 (10)
N4	0.1179 (5)	0.6611 (4)	0.6816 (3)	0.0696 (11)
C111	0.4621 (5)	0.3067 (4)	0.3857 (2)	0.0434 (8)
C112	0.2194 (7)	0.1464 (4)	0.2990 (3)	0.0591 (11)
C113	0.2189 (8)	0.0675 (5)	0.3634 (3)	0.0709 (13)
C114	0.3431 (7)	0.1108 (5)	0.4402 (3)	0.0699 (13)
C115	0.4727 (6)	0.2347 (4)	0.4533 (3)	0.0557 (10)
C116	0.6076 (7)	0.2900 (6)	0.5315 (3)	0.0682 (13)
C121	0.5869 (5)	0.4345 (4)	0.3962 (2)	0.0433 (8)
C122	0.6808 (6)	0.6214 (4)	0.3363 (3)	0.0543 (10)
C123	0.8154 (6)	0.6784 (5)	0.4112 (3)	0.0604 (11)
C124	0.8342 (6)	0.6115 (5)	0.4787 (3)	0.0596 (12)
C125	0.7193 (5)	0.4865 (4)	0.4730 (2)	0.0491 (9)
C126	0.7263 (7)	0.4092 (6)	0.5406 (3)	0.0634 (13)
C131	0.4485 (5)	0.3348 (3)	0.0548 (2)	0.0372 (8)
C132	0.7178 (5)	0.4662 (4)	0.1397 (3)	0.0505 (9)
C133	0.8051 (6)	0.4599 (5)	0.0696 (3)	0.0603 (12)
C134	0.7106 (6)	0.3862 (5)	−0.0093 (3)	0.0568 (11)
C135	0.5248 (5)	0.3200 (3)	−0.0183 (2)	0.0427 (8)
C136	0.4137 (6)	0.2397 (4)	−0.0982 (3)	0.0541 (10)
C141	0.2572 (5)	0.2711 (3)	0.0491 (2)	0.0378 (8)
C142	0.0142 (5)	0.2351 (4)	0.1171 (3)	0.0526 (10)
C143	−0.1007 (6)	0.1556 (4)	0.0421 (3)	0.0560 (10)
C144	−0.0336 (5)	0.1359 (4)	−0.0309 (3)	0.0507 (10)
C145	0.1514 (5)	0.1947 (3)	−0.0300 (2)	0.0428 (8)
C146	0.2357 (6)	0.1802 (4)	−0.1032 (3)	0.0522 (10)

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

Cu1—N15	1.984 (4)	C1—C2	1.387 (6)
Cu1—N12	1.987 (3)	C1—C3	1.400 (6)
Cu1—N14	2.000 (3)	C1—C4	1.395 (6)
Cu1—N11	2.078 (3)	C2—N2	1.147 (6)
Cu1—N13	2.112 (3)	C3—N3	1.143 (5)
N15—C15	1.137 (5)	C4—N4	1.145 (5)
C15—S15	1.612 (4)		
N15—Cu1—N12	92.76 (14)	N11—Cu1—N13	120.16 (12)
N15—Cu1—N14	93.17 (14)	C15—N15—Cu1	172.5 (3)
N12—Cu1—N14	173.95 (12)	N15—C15—S15	178.2 (4)
N15—Cu1—N11	126.62 (14)	C2—C1—C3	121.3 (4)
N12—Cu1—N11	80.81 (13)	C2—C1—C4	119.2 (4)
N14—Cu1—N11	96.58 (13)	C3—C1—C4	119.5 (4)
N15—Cu1—N13	113.19 (13)	N2—C2—C1	178.9 (6)
N12—Cu1—N13	96.04 (13)	N3—C3—C1	178.6 (5)
N14—Cu1—N13	80.49 (12)	N4—C4—C1	177.8 (4)

Intensities were corrected for Lorentz and polarization effects using *XP*21 (Pavelčík, 1993). The structure was solved by the heavy-atom method with *XFPS* (Pavelčík, Rizzoli & Andreetti, 1990) and subsequent Fourier syntheses using *SHELXL*93 (Sheldrick, 1993). Anisotropic displacement parameters were refined for all non-H atoms. All H atoms were located from the difference Fourier map and refined with free isotropic displacement parameters. Geometrical analysis was performed using *PARST* (Nardelli, 1983) and *SHELXL*93. *ORTEP* (Johnson, 1965) was employed to draw the structure.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1130). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Chloro(η^5-cyclopentadienyl)(triphenylphosphine)nickel(II)

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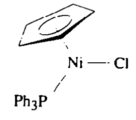
Abstract

The title compound, $[NiCl(C_5H_5)(C_{18}H_{15}P)]$, belongs to the class of two-legged piano-stool complexes, and has Ni—Cl and Ni—P distances of 2.176 (1) and 2.160 (1) Å, respectively.

Comment

We have been investigating the nonlinear optical responses of organometallic acetylides (Whittall *et al.*, 1994; Whittall, Humphrey, Hockless, Skelton & White, 1995). In the course of our studies employing *ZINDO* (Biosym Technologies, 1994) to compute molecular first hyperpolarizabilities, we have required accurate molecular geometries for acetylide complexes and their precursor chloro compounds. We report herein the structure determination of chloro(η^5-cyclopentadienyl)(triphenylphosphine)nickel(II), (I), which can be readily transformed into σ-arylacetylide derivatives by replacement of the chloro ligand (Bruce, Humphrey, Matisons, Roy & Swincer, 1984).



(I)

The title complex is readily obtained in excellent yield by ligand metathesis of $[Ni(\eta\text{-}C_5H_5)_2]$ and $[NiCl_2(PPh_3)_2]$ (Barnett, 1974), and can be crystallized from a toluene/hexane mixture. The Ni atom can be considered five-coordinate (with the cyclopentadienyl occupying three facially disposed sites). The complex is an example of a two-legged piano stool complex, of which many examples exist. The Ni—Cl [2.176 (1) Å], Ni—P [2.160 (1) Å] and Ni—C_5H_5 [2.081 (4)–2.154 (4) Å] distances fall within the range of expected values.

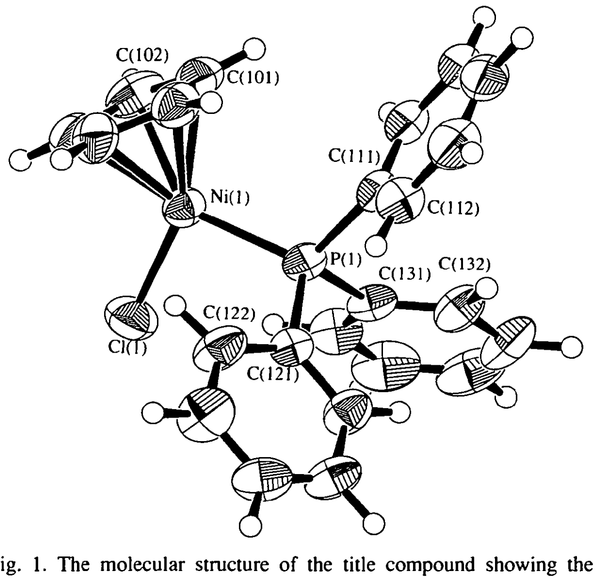


Fig. 1. The molecular structure of the title compound showing the labelling of the non-H atoms. Numbering of unlabelled atoms continues in sequence around each ring. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as circles of arbitrary radii.