Na2—O17	2.524 (3)	N4—C64	1.136 (6)
Na2—O12	2.572 (4)	C57—C58	1.396 (5)
Na2—O18	2.601 (4)	C58—C59	1.413 (6)
Na2—O14	2.768 (4)	C58—C60	1.431 (6)
Na2—O11	2.773 (4)	C61—C62	1.395 (5)
Na2—O16	2.937 (3)	C62—C64	1.400 (7)
Na2—O15	3.004 (3)	C62—C63	1.419 (6)
S1—C57	1.769 (4)		
C58—C57—S2	124.4 (3)	C62—C61—S4	113.0 (3)
C58—C57—S1	112.7 (3)	S3—C61—S4	123.5 (3)
S2—C57—S1	122.9 (2)	C61—C62—C64	123.2 (4)
C57—C58—C59	123.8 (4)	C61—C62—C63	121.1 (4)
C57—C58—C60	120.7 (4)	C64—C62—C63	115.8 (4)
C59—C58—C60	115.5 (4)	N3—C63—C62	177.2 (6)
N1—C59—C58	179.3 (5)	N4—C64—C62	178.0 (5)
N2—C60—C58	177.8 (5)	S4—C65—S1	116.0 (2)
C62—C61—S3	123.5 (3)		

Data were collected with a scan speed of <7.00° min^{-1} and a scan width of $(0.60 + 0.35\tan\theta)^\circ$ (in ω). The structure was solved by direct methods. The Na atom was located in the *E* map and the remaining non-H atoms were deduced from successive Fourier syntheses. The structure was refined by full-matrix least-squares techniques. H atoms were positioned geometrically and not refined. All calculations were performed on a PC 486 computer.

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

This research was supported by grants from the National Science Foundation of China.

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: KH1122). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bush, M. A. & Truter, M. R. (1972). *J. Chem. Soc. Perkin Trans.* 2, pp. 341–344.
Dreissig, W., Dauter, Z., Cygan, A. & Biernat, J. F. (1985). *Inorg. Chim. Acta*, **96**, 21–27.
Hummel, H.-U. (1987). *Acta Cryst.* C**43**, 41–43.
Hummel, H.-U. & Meske, H. (1989). *J. Chem. Soc. Dalton Trans.* pp. 627–640.
Li, H. Y. & Amma, E. L. (1990). *Inorg. Chim. Acta*, **177**, 5–7.
Long, D. L., Hou, H. W., Xin, X. Q., Yu, K. B., Luo, B. S. & Chen, L. R. (1996). *J. Coord. Chem.* **38**, 15–24.
Moody, D. C. & Ryan, R. R. (1979). *Cryst. Struct. Commun.* **8**, 933–936.
Owen, J. D. (1980). *J. Chem. Soc. Dalton Trans.* pp. 1066–1075.
Sheldrick, G. M. (1990). *SHELXTL/PC Users Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
Siemens (1994*a*). *XSCANS. X-ray Single-Crystal Analysis System*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1994*b*). *SHELXTL Reference Manual*. Version 5.0. Siemens Analytical X-ray Instruments Inc., Madison, Wiscosin, USA.
Ward, D. L., Popov, A. I. & Poonia, N. S. (1984). *Acta Cryst.* C**40**, 238–241.

Acta Cryst. (1997). C**53**, 556–559

Bis[(1,1,2,3,3-pentacyanopropenido-N^1:N^2)-bis(triphenylphosphine-*P*)copper(I)]

ANDREJ DVORSKÝ,[a] JOZEF KOŽÍŠEK,[a] LOTHAR JÄGER[b] AND CAROLA TRETNER[b]

[a]*Department of Inorganic Chemistry, Faculty of Chemical Technology, Radlinského 9, Slovak Technical University, 812 37 Bratislava, Slovakia, and* [b]*Institute of Inorganic Chemistry, Martin-Luther-University Halle-Wittenberg, D-06099 Halle/Saale, Germany. E-mail: dvorsky@cvtstu.cvt.stuba.sk*

(*Received 30 May 1996; accepted 9 December 1996*)

Abstract

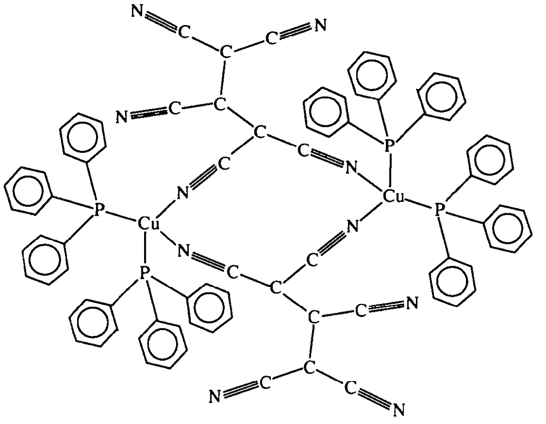
The title complex, $[Cu(C_8N_5)(C_{18}H_{15}P)_2]_2$, is a dimer. The two Cu atoms are bridged by the $C(CN)_2$ units of the pentacyanopropenide moiety. The coordination polyhedron of the Cu^I atoms is a distorted tetrahedron with a CuN_2P_2 chromophore.

Comment

In connection with our investigations on the ambidentate behaviour of $C(CN)_2$-modified derivatives of inorganic oxoacids, we have been interested in the coordination behaviour of pentacyanopropenide towards singly charged metal ions. Discussing the fragments $C(CN)_2$ and CCN as pseudo-chalcogen or pseudo-pnictogen (Jäger & Köhler, 1992), the ions NO_2^-, $[NOC(CN)_2]^-$, $[N\{C(CN)_2\}_2]^-$ and $[NCC\{C(CN)_2\}_2]^-$ can be considered as a homologous series.

Depending on the character of the metal atom, dicyanomethanidonitrite, like nitrite, forms coordinative bonds through the central N (Re^I; Fritsch, Polborn, Sünkel, Beck, Köhler & Jäger, 1992) or O atom (Cu^{II}; Hvastijová, Kožíšek, Kohout, Mroziński, Jäger & Svoboda, 1997). On the other hand, from $[N\{C(CN)_2\}_2]^-$ we know complexes in which the ionic ligand is coordinated exclusively through the terminal N atom (Cu^I, Ag^I; Jäger & Tretner, 1997). To the best of our knowledge, for $[NCC\{C(CN)_2\}_2]^-$ only the structure of $[CuCl(bipy)_2][NCC\{C(CN)_2\}_2]$ (Jensen & Jakobson, 1981) has been described. Here, the corresponding ligand exists as an uncoordinated counterion. For $[NCC\{C(CN)_2\}_2]^-$, quantum-chemical investigations predict coordinative bonds *via* terminal N atoms of the $C(CN)_2$ groups. Coordination *via* the central nitrile group end seems to be rather improbable (Jäger, Schädler, Grobe, Köhler & Nefedov, 1992). The title compound, (I), consists of discrete dimeric units.

Acta Crystallographica Section C
ISSN 0108-2701 © 1997



(I)

The nearly planar pentacyanopropenide acts as a bidentate bridging ligand with bonds to both Cu atoms through the terminal N atoms of one $C(CN)_2$ group (Fig. 1). The geometry of the ligands about copper is that of a strongly distorted tetrahedron with two P and two N atoms. The P atoms occupy positions above and below the plane formed by the two pentacyanopropenide ligands. As a result of different steric demands, the angle P1—Cu—P2 [126.55 (4)°] is much larger than N1—Cu—N2^{i} [92.8 (1)°; symmetry code: (i) $-x$, $-y$, $-z$].

The Cu—P distances of 2.241 (1) and 2.274 (1) Å are in fairly good agreement with similar bond lengths found in $[Cu(NO_2)(PPh_3)_2]$ (2.243 Å; Halfen & Tolman, 1995) and $[Cu(NO_3)(PPh_3)_2]$ (2.256 Å; Messmer & Palink, 1969). The distances to the N atoms of 2.010 (3) and 2.064 (3) Å are normal for this type of bond (Cu^{I}, coordination number 4, nitrile group; Orpen, Brammer, Allen, Kennard, Watson & Taylor, 1989).

The uncoordinated part of the ionic ligand – one $C(CN)_2$ and the central nitrile group – is disordered. The C—N distances of coordinated as well as of uncoordinated nitrile groups correspond with the standard value (C—N 1.15 Å; Rademacher, 1987). For the bonds of the central C4*A* atom to the neighbouring C2 and C5*A* atoms [1.387 (7) and 1.366 (8) Å, respectively], as well as in the disordered part for C4*B* bonded to C2 and C5*B* [1.436 (7) and 1.364 (9) Å], a bonding order of about 1.5 can be assumed. As expected from the point of view of the charge distribution in this ion (Jäger, Schädler, Grobe, Köhler & Nefedov, 1992), the distances C4*A*—C6*A* [1.513 (9) Å] and C4*B*—C6*B* [1.490 (9) Å] are significantly longer. The distances C2—C1 [1.412 (5) Å]

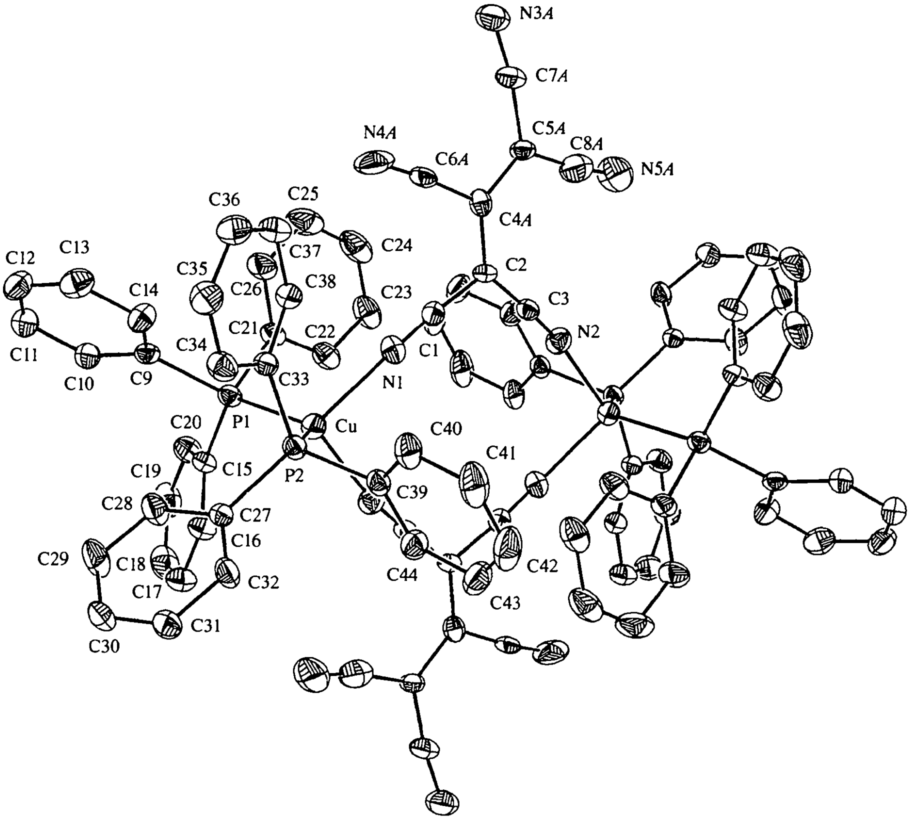


Fig. 1. The structure of compound (I) showing 50% probability displacement ellipsoids. The disordered part *B* and the H atoms have been omitted for clarity.

and C2—C3 [1.406 (5) Å] are somewhat shortened in comparison with a single bond of the type C_{sp}—C_{sp^2} of 1.432 Å.

The angles within the $C(CN)_2$ groups are C3—C2—C1 114.6 (3)° (coordinated), and C7*A*—C5*A*—C8*A* 118.3 (7) and C7*B*—C5*B*—C8*B* 119.0 (8)° (uncoordinated). The angles C3—C2—C4*A* and C1—C2—C4*A* of 133.1 (3) and 112.3 (3)°, respectively, are similar to C1—C2—C4*B* and C3—C2—C4*B* [133.3 (3) and 112.0 (3)°, respectively]. On the other hand, the corresponding angles of the uncoordinated part of the ligands are rather similar [119.8 (7)–121.8 (7)°].

Experimental

$K[NCC\{C(CN)_2\}_2]$ (1 mmol, 0.21 g) (Middleton, Little, Coffman & Engelhardt, 1958) was dissolved in 10 ml methanol and added to a solution of $[Cu(NO_3)(PPh_3)_2]$ (1 mmol, 0.63 g) (Gysling & Kubas, 1976) in 15 ml $CHCl_3$. The mixture was heated to reflux for 1 h in a water bath and then filtered. After evaporation of the solvent, the resulting solid was washed with methanol. To a solution of the crude product in chloroform, *n*-hexane was added until the solution became cloudy, whereupon it was cooled for a few hours yielding a microcrystalline product (91%, 0.69 g). Single crystals are obtained by dissolving 0.5 g of the product in 2 ml $CHCl_3$ in a test tube and carefully overlaying with 6 ml petroleum ether. ^{31}P NMR (in $CHCl_3$, D_2O-containing capillary): δ 0.03 p.p.m.; IR (KBr): ν(CN) 2205 (*vs*) cm^{-1}. Calculated for $C_{88}H_{60}Cu_2N_{10}P_2$: M_r 1508.5, C 70.07 (found 68.57), H 4.04 (4.03), N 9.29% (9.27)%.

Crystal data

$[Cu_2(C_8N_5)_2(C_{18}H_{15}P)_4]$
M_r = 1508.42
Monoclinic
$P2_1/n$
a = 13.798 (5) Å
b = 20.533 (9) Å
c = 13.850 (6) Å
β = 104.50 (3)°
V = 3799 (3) $Å^3$
Z = 2
D_x = 1.319 Mg m^{-3}
D_m = 1.31 (3) Mg m^{-3}
D_m measured by flotation in nitrobenzene and CCl_4

Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 22 reflections
θ = 4.0–9.9°
μ = 0.697 mm^{-1}
T = 293 (2) K
Prism
0.55 × 0.35 × 0.15 mm
Dark yellow

Data collection

Syntex $P2_1$ four-circle diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical *via* ψ scan (North, Phillips & Mathews, 1968)
T_{min} = 0.545, T_{max} = 0.901
6776 measured reflections
6776 independent reflections

3427 reflections with $I > 2\sigma(I)$
θ_{max} = 27.57°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 26$
$l = -18 \rightarrow 17$
2 standard reflections every 98 reflections intensity decay: 15%

Refinement

Refinement on F^2
$R(F)$ = 0.0436
$wR(F^2)$ = 0.1034
S = 0.907
6775 reflections
542 parameters
H atoms not refined
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = −0.157
$\Delta\rho_{max}$ = 0.334 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.201 e $Å^{-3}$
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

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}
Cu	0.06857 (4)	0.13340 (2)	0.15851 (3)	0.0502 (2)
P1	0.06174 (8)	0.09094 (5)	0.30827 (6)	0.0478 (3)
P2	0.09961 (8)	0.23738 (4)	0.12718 (6)	0.0457 (3)
C9	0.0368 (3)	0.1426 (2)	0.4049 (2)	0.0493 (10)
C10	0.0642 (3)	0.1272 (2)	0.5053 (3)	0.0633 (11)
C11	0.0429 (3)	0.1690 (3)	0.5742 (3)	0.0811 (14)
C12	−0.0052 (4)	0.2257 (3)	0.5466 (3)	0.0834 (14)
C13	−0.0310 (3)	0.2421 (2)	0.4481 (4)	0.0827 (14)
C14	−0.0094 (3)	0.2005 (2)	0.3782 (3)	0.0693 (12)
C15	0.1669 (3)	0.0420 (2)	0.3716 (2)	0.0514 (10)
C16	0.2594 (4)	0.0588 (2)	0.3601 (3)	0.0690 (13)
C17	0.3442 (4)	0.0248 (3)	0.4093 (4)	0.090 (2)
C18	0.3345 (5)	−0.0266 (3)	0.4683 (4)	0.103 (2)
C19	0.2436 (5)	−0.0449 (2)	0.4797 (3)	0.089 (2)
C20	0.1594 (3)	−0.0112 (2)	0.4312 (3)	0.0684 (12)
C21	−0.0410 (3)	0.0345 (2)	0.2792 (2)	0.0530 (11)
C22	−0.0330 (3)	−0.0211 (2)	0.2269 (3)	0.0665 (12)
C23	−0.1137 (5)	−0.0606 (2)	0.1880 (3)	0.084 (2)
C24	−0.2045 (5)	−0.0441 (3)	0.2015 (4)	0.094 (2)
C25	−0.2165 (4)	0.0106 (3)	0.2521 (4)	0.099 (2)
C26	−0.1334 (4)	0.0500 (2)	0.2921 (3)	0.0761 (14)
C27	0.2131 (3)	0.2706 (2)	0.2065 (2)	0.0426 (9)
C28	0.2331 (3)	0.2601 (2)	0.3068 (3)	0.0713 (13)
C29	0.3162 (4)	0.2856 (2)	0.3702 (3)	0.087 (2)
C30	0.3819 (3)	0.3209 (2)	0.3350 (3)	0.0764 (13)
C31	0.3637 (3)	0.3325 (2)	0.2365 (3)	0.0817 (14)
C32	0.2796 (3)	0.3074 (2)	0.1726 (3)	0.0695 (13)
C33	0.0039 (3)	0.2943 (2)	0.1406 (2)	0.0448 (10)
C34	0.0227 (3)	0.3599 (2)	0.1617 (3)	0.0643 (12)
C35	−0.0552 (4)	0.4013 (2)	0.1628 (3)	0.0800 (15)
C36	−0.1501 (4)	0.3790 (3)	0.1433 (3)	0.0827 (15)
C37	−0.1693 (4)	0.3144 (3)	0.1257 (3)	0.0770 (14)
C38	−0.0917 (4)	0.2728 (2)	0.1253 (2)	0.0552 (11)
C39	0.1133 (3)	0.2541 (2)	0.0029 (2)	0.0497 (10)
C40	0.0608 (3)	0.3012 (2)	−0.0583 (3)	0.0721 (13)
C41	0.0781 (4)	0.3124 (3)	−0.1517 (3)	0.098 (2)
C42	0.1459 (5)	0.2760 (3)	−0.1837 (4)	0.107 (2)
C43	0.1980 (4)	0.2283 (3)	−0.1244 (3)	0.089 (2)
C44	0.1806 (3)	0.2170 (2)	−0.0319 (3)	0.0687 (12)
N1	−0.0646 (3)	0.10234 (15)	0.0655 (2)	0.0576 (9)
N2	−0.1492 (3)	−0.0677 (2)	−0.1044 (2)	0.0640 (10)
C1	−0.1311 (3)	0.0726 (2)	0.0230 (2)	0.0487 (11)
C2	−0.2100 (3)	0.0339 (2)	−0.0329 (2)	0.0472 (10)
C3	−0.1790 (3)	−0.0223 (2)	−0.0748 (2)	0.0487 (10)
C4*A*†	−0.3034 (5)	0.0592 (3)	−0.0334 (4)	0.049 (2)
C5*A*†	−0.3940 (6)	0.0334 (3)	−0.0808 (5)	0.057 (2)
C6*A*†	−0.3097 (5)	0.1210 (4)	0.0242 (5)	0.062 (2)
C7*A*†	−0.4848 (6)	0.0609 (4)	−0.0709 (6)	0.072 (3)
C8*A*†	−0.3984 (7)	−0.0251 (5)	−0.1379 (7)	0.097 (3)
N3*A*†	−0.5568 (5)	0.0825 (4)	−0.0511 (5)	0.088 (3)
N4*A*†	−0.3056 (5)	0.1667 (4)	0.0720 (5)	0.100 (3)
N5*A*†	−0.4116 (6)	−0.0677 (4)	−0.1799 (6)	0.128 (4)
C4*B*‡	−0.3171 (5)	0.0385 (3)	−0.0537 (5)	0.049 (2)
N3*B*‡	−0.2898 (6)	0.1633 (4)	0.1083 (5)	0.094 (3)
N4*B*‡	−0.4249 (5)	−0.0397 (4)	−0.1897 (6)	0.106 (3)
N5*B*‡	−0.5618 (5)	0.0881 (4)	−0.0822 (5)	0.089 (3)
C5*B*‡	−0.3688 (6)	0.0856 (4)	−0.0184 (5)	0.065 (2)

C6*B*‡	−0.3814 (6)	−0.0063 (4)	−0.1273 (6)	0.066 (2)
C7*B*‡	−0.3204 (6)	0.1269 (5)	0.0558 (6)	0.078 (3)
C8*B*‡	−0.4777 (8)	0.0858 (4)	−0.0480 (6)	0.084 (3)

† Site occupancy = 0.501 (2). ‡ Site occupancy = 0.499 (2).

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

Cu—N2^{i}	2.010 (3)	N2—C3	1.135 (4)
Cu—N1	2.064 (3)	N2—Cu^{i}	2.010 (3)
Cu—P2	2.2412 (13)	C1—C2	1.412 (5)
Cu—P1	2.2735 (13)	C2—C3	1.406 (5)
N1—C1	1.137 (4)		
N2^{i}—Cu—N1	92.81 (13)	C1—N1—Cu	165.2 (3)
N2^{i}—Cu—P2	114.64 (10)	C3—N2—Cu^{i}	166.0 (3)
N1—Cu—P2	110.91 (9)	N1—C1—C2	176.6 (4)
N2^{i}—Cu—P1	103.67 (10)	C3—C2—C1	114.6 (3)
N1—Cu—P1	102.55 (9)	N2—C3—C2	176.1 (4)
P2—Cu—P1	126.55 (4)		

Symmetry code: (i) $-x, -y, -z$.

The disordered part of the structure could be described as the rotation around a twofold axis defined through atom C2 and the midpoint of the N3*A* and N3*B* atoms. Because of the disorder overlap, it was not possible to refine the atom sites free of constraints. Each disordered atom was modelled as a pair of separated atoms with the sum of the population constrained to 1.0. The sites were obtained by careful splitting of the atomic positions which were found in a difference map. After this, the structure was refined in two blocks (the disordered and the undisordered part). Displacement parameters were refined anisotropicaly without constraints, but separately from refinement of positional parameters. All H atoms were introduced at calculated positions (C—H 0.93 Å) and refined in the riding mode with isotropic displacement parameters $1.2U_{eq}$ of their carrier atoms.

Data collection: Syntex *P*2$_1$ software. Cell refinement: Syntex *P*2$_1$ software. Data reduction: *XP*21 (Pavelčík, 1993). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1971). Software used to prepare material for publication: *SHELXL*93.

This work was supported by Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie.

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: SK1037). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Fritsch, E., Polborn, K., Sünkel, K., Beck, W., Köhler, H. & Jäger, L. (1992). *Z. Anorg. Allg. Chem.* **617**, 110–116.
Gysling, H. J. & Kubas, G. J. (1976). *Inorg. Synth.* **16**, 92–97.
Halfen, J. A. & Tolman,W. B. (1995). *Acta Cryst.* **C51**, 215–218.
Hvastijová, M., Kožíšek, J., Kohout, J., Mroziński, J., Jäger, L. & Svoboda, I. (1997). *Polyhedron*, **17**, 463–471.
Jäger, L. & Köhler, H. (1992). *Sulfur Rep.* **12**, 159–212.
Jäger, L., Schädler, H.-D., Grobe, U., Köhler, H. & Nefedov, V. I. (1992). *Z. Anorg. Allg. Chem.* **617**, 123–126.
Jäger, L. & Tretner, C. (1997). Unpublished results.
Jensen, W. P. & Jakobson, R. A. (1981). *Inorg. Chim. Acta*, **50**, 189–194.
Johnson, C. K. (1971). *ORTEP*II. Report ORNL-3794, revised. Oak Ridge National Laboratory, Tennessee, USA.
Messmer, G. G. & Palink, G. J. (1969). *Inorg. Chem.* **8**, 2750–2754.
Middleton, W. J., Little, E. L., Coffman, D. D. & Engelhardt, V. A. (1958). *J. Am. Chem. Soc.* **80**, 2795–2806.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1–S83.
Pavelčík, F. (1993). *XP*21. *Program for Syntex P*2$_1$ *Data Reduction.* Comenius University, Bratislava, Slovakia.
Rademacher, P. (1987). *Strukturen organischer Moleküle*, p. 56. Weinheim: VCH.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.

Acta Cryst. (1997). **C53**, 559-562

Two TEPA–Copper(II) Complexes {TEPA is Tris[2-(2-pyridyl)ethyl]amine}

El Houssine Alilou,[a] Abdelilah El Hallaoui,[a] El Houssine El Ghadraoui,[a] Michel Giorgi,[b] Marcel Pierrot[b] and Marius Réglier[b]

[a]*Faculté des Sciences et Techniques Fès Sais, Université Sidi Mohamed ben Abdellah, BP 2202, Fès, Morroco, and* [b]*Laboratoire de Bioinorganique Structurale, Faculté des Sciences et Techniques de Saint Jérôme, Avenue Escadrille Normandie Niemen, 13397 Marseille CEDEX 20, France. E-mail: mpie@ms432u04.u-3mrs.fr*

(*Received 15 October 1996; accepted 9 December 1996*)

Abstract

In both the title compounds, aqua{tris[2-(2-pyridyl)-ethyl]amine-*N*,*N'*,*N''*,*N'''*}copper(II) bis(trifluoromethanesulfonate) monohydrate, $[Cu(C_{21}H_{24}N_4)(H_2O)](CF_3SO_3)_2.H_2O$, (1), and (acetato-*O*){tris[2-(2-pyridyl)-ethyl]amine-*N*,*N'*,*N''*,*N'''*}copper(II) hexafluorophosphate, $[Cu(C_2H_3O_2)(C_{21}H_{24}N_4)]PF_6$, (2), the Cu^{II} atom is pentacoordinate and the geometry is described as square-based pyramidal. Three of the atoms in the equatorial plane remain unchanged, *i.e.* N1, N2 and N3 from the tripodal amine and two pyridine groups, respectively, while the fourth ligand is a water molecule in (1) and an acetate group in (2). The axial position is occupied in both cases by the N4 atom of the third pyridine ring.

Comment

Our work on the functional modeling of copper proteins (Réglier, Amadéi, Tadayoni & Waegell, 1989; Réglier, Jorand & Waegell, 1990; Alilou, Giorgi, Pierrot & Réglier, 1992; Amadéi, Alilou, Eydoux, Pierrot, Réglier & Waegell, 1992; Alilou, Amadéi, Pierrot & Réglier, 1993; Réglier, Amadéi, Alilou, Eydoux, Pierrot