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{5-[4′-(2,2,5,5-Tetramethyl-3-pyrroline-1-oxyl-3-carbonyl)biphenyl-4-ylethynyl]-2,3,7,8,12,13,17,18-octaethylporphyrinato}copper(**II**) benzene solvate. Corrigendum

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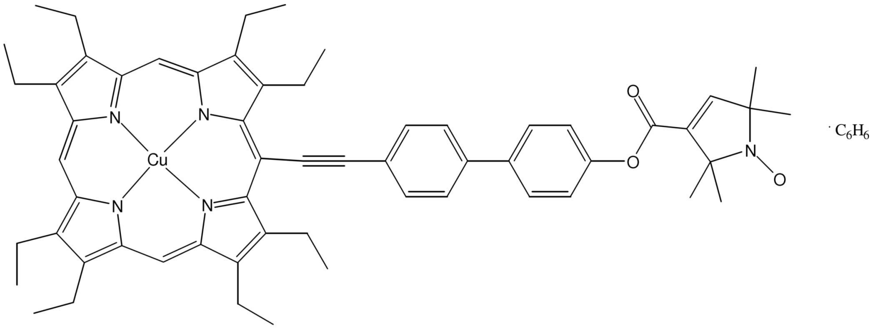
In the paper by Bolte [*Acta Cryst.* (2006), E**62**, m1609–m1610], the chemical name in the title and the chemical diagram are incorrect. The correct title is '{5-[4′-(2,2,5,5-Tetramethyl-3-pyrroline-1-oxyl-3-carbonyloxy)biphenyl-4-ylethynyl]-2,3,7,8,-12,13,17,18-octaethylporphyrinato}copper(II) benzene solvate' and the correct diagram is given below.



(I)

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Key indicators

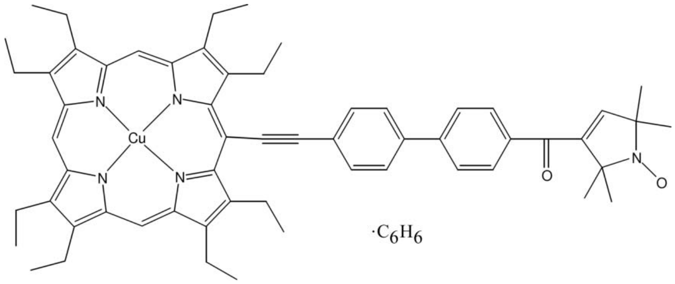
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.051
wR factor = 0.119
Data-to-parameter ratio = 15.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{59}H_{64}CuN_5O_3\cdot C_6H_6$, features an essentially planar porphyrin ring system, with the Cu atom located in the plane and showing equal Cu—N distances. The space between the molecules is occupied by benzene solvent molecules.

Comment

The title compound, (I), was prepared for use in distance measurements by electron paramagnetic resonance spectroscopy (Plackmeyer, 2006). The intramolecular distance in question, between the Cu atom and the nitroxide O atom, is 21.254 (3) Å, which is much longer than the shortest intermolecular Cu1···O74^{i} distance of 8.050 (3) Å [symmetry code: (i) $2 - x$, $2 - y$, $-z$].



(I)

Bond lengths and angles show normal values (Cambridge Structural Database, Version 5.27, updated May 2006; *MOGUL* Version 1.1; Allen, 2002). The porphyrin ring system is essentially planar (r.m.s. deviation for all core non-H atoms = 0.213 Å). The Cu atom deviates only insignificantly [0.0809 (6) Å] from this plane. The Cu—N distances are almost equal (Table 1). The C53–C58 benzene ring makes a dihedral angle of 41.02 (8)° with the porphyrin plane. The dihedral angle between the two benzene rings is 29.76 (10)°. The pyrroline ring is planar (r.m.s. deviation for all non-H atoms = 0.0034 Å) and coplanar with the ester group to which it is attached (Table 1). The dihedral angle between the pyrroline ring and the C61—C66 benzene ring is 77.59 (10)°.

The molecules pack in sheets perpendicular to [$\bar{2}$12], with the benzene molecules filling the space between them.

Experimental

The synthesis and electron paramagnetic resonance measurements of the title compound will be described elsewhere (Plackmeyer, 2006). Crystals of (I) for X-ray analysis were obtained by recrystallization from benzene.

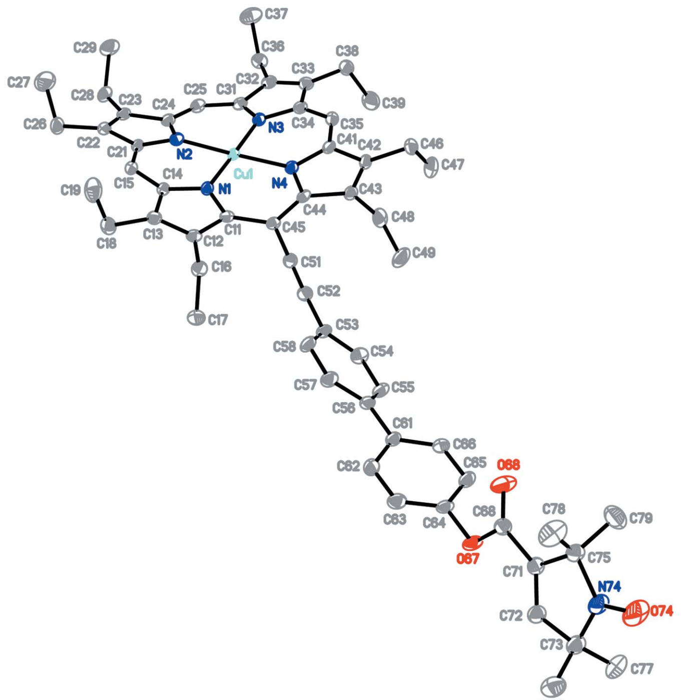


Figure 1
A perspective view of the title compound, with the atom numbering. Displacement ellipsoids are drawn at the 50% probability level. H atoms and the solvent benzene molecule have been omitted for clarity.

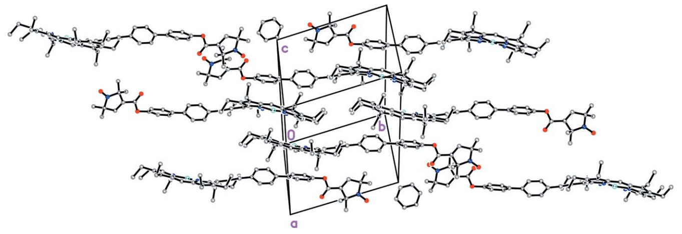


Figure 2
A packing diagram for (I), viewed approximately along $[\bar{1}0\bar{1}]$. H atoms have been omitted.

Crystal data

$C_{59}H_{64}CuN_5O_3 \cdot C_6H_6$
$M_r = 1032.80$
Triclinic, $P\bar{1}$
$a = 12.7494$ (8) Å
$b = 13.1040$ (8) Å
$c = 17.4594$ (11) Å
$\alpha = 73.325$ (5)°
$\beta = 82.552$ (5)°
$\gamma = 89.157$ (5)°
$V = 2769.9$ (3) Å^3
$Z = 2$
$D_x = 1.238$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.45$ mm^{-1}
$T = 173$ (2) K
Plate, red
0.24 × 0.13 × 0.08 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{\min} = 0.901$, $T_{\max} = 0.945$
35264 measured reflections
10306 independent reflections
7700 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.097$
$\theta_{\max} = 25.6°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.119$
$S = 1.00$
10306 reflections
667 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.55$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	2.004 (2)	C51—C52	1.211 (4)
Cu1—N1	2.008 (2)	C73—N74	1.487 (4)
Cu1—N4	2.008 (2)	N74—O74	1.278 (3)
Cu1—N3	2.009 (2)	N74—C75	1.483 (4)
O68—C68—C71—C72	177.5 (3)	O67—C68—C71—C75	178.0 (2)

All H atoms were positioned geometrically, with C—H distances in the range 0.95–0.99 Å, and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C), or 1.5$U_{\rm eq}$(C$_{\rm methyl}$).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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