

Fig. 3. A unit cell (ORTEP; Johnson, 1976) of the title compound. Li⁺ ions are filled; Li—O coordination is represented by dashed lines. One formula unit is shown within the central portion of the cell while four additional asymmetric units are shown outside the cell.

and below the naphthalene rings is occupied by water molecules; altogether, the water molecules participate in a three-dimensional network of hydrogen bonds. The two water molecules not involved in coordination of Li⁺ ions supplement the packing around the naphthalene ring.

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The Structure of Copper(II) 5,7,12,14-Tetramethyldibenzo[*b*,*d*][1,4,8,11]-tetraazacyclotetradeca-2,4,7,9,11,14-hexaenediide*

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Abstract. [Cu(C₂₂H₂₂N₄)], *M_r* = 405.99, monoclinic, *P*2₁/*c*, *a* = 14.318 (2), *b* = 16.427 (2), *c* = 16.299 (2) Å, β = 100.01 (1)°, *V* = 3775 (1) Å³, *Z* = 8, *D_x* = 1.429 g cm⁻³, λ(Cu *K*α) = 1.54183 Å, μ = 16.88 cm⁻¹, *F*(000) = 1688, *T* = 296 K, *R* = 0.0355, 4237 unique observations with *I* > 3σ(*I*). There are two crystallographically independent molecules but they are virtually identical. Each has the ligand, tmtaa, in a flattened saddle conformation, whereby the Cu ion can have nearly planar coordination. The

Cu—N distances range from 1.922 (2) to 1.948 (2) Å with a mean value of 1.930 Å.

Introduction. The coordination chemistry of the title macrocyclic ligand has recently been reviewed (Cotton & Czuchajowska, 1990*a*). It is well established that, because of the small size of the 'hole' together with a tendency to minimize internal non-bonded repulsions, this ligand characteristically adopts a saddle shape. This, in turn, causes the metal ion to sit above the plane of the four N atoms. Only two exceptions to this have been reported, namely [Ru(tmtaa)(PMePh₂)₂] (Cotton & Czuchajowska, 1990*b*) and [Pd(tmtaa)] (Tsutsui, Bobsein, Cash &

* IUPAC name: {6,8,15,17-tetramethyl-7*H*,16*H*-5,9,14,18-tetraazadibenzo[*b*,*d*]cyclotetradecanato(2-)-κ⁴N,N',N'',N'''}copper(II).

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Pettersen, 1979). In these two cases the tmtaa ligands adopt a step geometry that creates a center of inversion at the midpoint of a truly planar rectangular (nearly square) set of N atoms. The explanation suggested for the occurrence of this exceptional ligand conformation in the former compound was that repulsive forces between the phenyl groups of the P₂MePh₂ ligands above and below the [Ru(tmtaa)] moiety impose it whereas, in the latter case, the strong tendency of Pd^{II} to prefer square coordination was held responsible.

Since the ability of the tmtaa ligand to adopt the centrosymmetric conformation in response to sufficient constraint or demand is thus established, we wondered if the well known tendency of the Cu^{II} ion to have square coordination would again lead to the occurrence of this conformation. The preparation of the compound, [Cu(tmtaa)], had already been reported (Jager, 1969; Woodruff, Pastor & Dabrowiak, 1976) but the structure was unknown. We report the structure here and show that it still contains a saddle-shaped ligand, but with the metal atom in the most nearly planar coordination yet observed.

Experimental. The complex was synthesized under a dry argon atmosphere by refluxing a solution of [Cu(O₂CCH₃)₂].H₂O (0.05 g, 0.25 mmol) and H₂tmtaa (0.09 g, 0.25 mmol) in toluene (16 ml) for about 20 h. The final emerald green solution was cooled to room temperature, filtered through Celite and layered with 25 ml of isomeric *n*-hexanes. A plentiful crop of nicely formed dark green crystals along with some green precipitate collected on the bottom of the Schlenk tube within 48 h. Yield: 0.070 g (ca 70%).

A block-like crystal of the sample, 0.2 × 0.3 × 0.3 mm, was coated with epoxy cement and mounted on the goniometer head of a Rigaku AFC5R diffractometer. 24 diffraction vectors were used in the determination of the orientation matrix and lattice dimensions. The set was well spread in space and spanned a 2θ range of roughly 43.0 to 50.0°. Indexing revealed a monoclinic cell and Laue symmetry *m* was confirmed by an oscillation photograph. The data were collected with a constant speed of 8° min⁻¹ in ω. Each scan was repeated four times or until *F*/σ(*F*) reached 30, whichever came first. The data were collected to 115° in 2θ. The intensities of the standard reflections 246, 208 and 228 varied by < 2%. Of the 5608 reflections collected in the +*h*, +*k* quadrant, 5386 were unique. *R*_{int} = 0.013. Data were corrected for Lorentz and polarization effects (Sheldrick, 1986) and absorption (North, Phillips & Matthews, 1968). The empirical absorption correction made was based on ψ scans of several reflections with χ near 90°; transmission coefficients were 0.770

Table 1. *Positional parameters and their e.s.d.'s for [Cu(tmtaa)]*

$$B_{eq} = (1/3) \sum_i \sum_j B_{ij} a_i^* a_j^* a_i a_j$$

	x	y	z	<i>B</i> _{eq} (Å ²)
Cu(1)	0.18173 (3)	0.01748 (2)	0.09181 (2)	2.989 (8)
Cu(2)	0.29821 (3)	0.00022 (2)	0.37666 (2)	2.924 (8)
N(1)	0.2163 (1)	0.1257 (1)	0.1357 (1)	3.10 (5)
N(2)	0.2732 (2)	0.0156 (1)	0.0178 (1)	3.28 (5)
N(3)	0.1431 (2)	-0.0869 (1)	0.0422 (1)	3.29 (5)
N(4)	0.0835 (2)	0.0244 (1)	0.1585 (1)	3.19 (5)
N(5)	0.3682 (2)	0.0289 (1)	0.2902 (1)	3.16 (5)
N(6)	0.2245 (2)	-0.0842 (1)	0.3137 (1)	3.18 (5)
N(7)	0.2321 (2)	-0.0334 (1)	0.4644 (1)	3.35 (5)
N(8)	0.3806 (2)	0.0764 (1)	0.4434 (1)	3.17 (5)
C(1)	0.2551 (2)	0.1805 (2)	0.0926 (2)	3.36 (6)
C(2)	0.2942 (2)	0.1590 (2)	0.0221 (2)	3.75 (6)
C(3)	0.3025 (2)	0.0835 (2)	-0.0141 (2)	3.49 (6)
C(4)	0.2857 (2)	-0.0646 (2)	-0.0102 (2)	3.41 (6)
C(5)	0.3637 (2)	-0.0922 (2)	-0.0415 (2)	4.34 (7)
C(6)	0.3709 (2)	-0.1730 (2)	-0.0630 (2)	5.15 (8)
C(7)	0.3034 (3)	-0.2274 (2)	-0.0503 (2)	5.19 (8)
C(8)	0.2266 (2)	-0.2024 (2)	-0.0158 (2)	4.46 (7)
C(9)	0.2151 (2)	-0.1202 (2)	0.0034 (2)	3.47 (6)
C(10)	0.0549 (2)	-0.1142 (2)	0.0365 (2)	3.56 (6)
C(11)	-0.0105 (2)	-0.0785 (2)	0.0806 (2)	3.67 (6)
C(12)	0.0015 (2)	-0.0140 (2)	0.1373 (2)	3.47 (6)
C(13)	0.1041 (2)	0.0853 (2)	0.2202 (2)	3.33 (6)
C(14)	0.0676 (2)	0.0900 (2)	0.2937 (2)	4.34 (7)
C(15)	0.0980 (3)	0.1496 (2)	0.3512 (2)	5.30 (8)
C(16)	0.1681 (2)	0.2031 (2)	0.3396 (2)	5.04 (8)
C(17)	0.2085 (2)	0.1972 (2)	0.2694 (2)	4.33 (7)
C(18)	0.1771 (2)	0.1406 (2)	0.2079 (2)	3.26 (6)
C(19)	0.2556 (2)	0.2700 (2)	0.1114 (2)	4.64 (7)
C(20)	0.3411 (2)	0.0841 (2)	-0.0943 (2)	5.33 (8)
C(21)	0.0162 (2)	-0.1829 (2)	-0.0204 (2)	4.85 (8)
C(22)	-0.0865 (2)	0.0118 (2)	0.1700 (2)	4.49 (7)
C(23)	0.3821 (2)	-0.0236 (2)	0.2318 (2)	3.43 (6)
C(24)	0.3289 (2)	-0.0947 (2)	0.2156 (2)	3.68 (6)
C(25)	0.2542 (2)	-0.1247 (2)	0.2528 (2)	3.41 (6)
C(26)	0.1437 (2)	-0.1028 (2)	0.3486 (2)	3.28 (6)
C(27)	0.0603 (2)	-0.1358 (2)	0.3066 (2)	4.02 (6)
C(28)	-0.0193 (2)	-0.1413 (2)	0.3436 (2)	4.78 (7)
C(29)	-0.0157 (2)	-0.1124 (2)	0.4233 (2)	4.88 (7)
C(30)	0.0663 (2)	-0.0789 (2)	0.4659 (2)	4.24 (7)
C(31)	0.1476 (2)	-0.0742 (2)	0.4312 (2)	3.36 (6)
C(32)	0.2720 (2)	-0.0283 (2)	0.5444 (2)	3.97 (7)
C(33)	0.3520 (2)	0.0187 (2)	0.5713 (2)	4.08 (7)
C(34)	0.4034 (2)	0.0692 (2)	0.5260 (2)	3.43 (6)
C(35)	0.4255 (2)	0.1284 (2)	0.3929 (2)	3.20 (6)
C(36)	0.4672 (2)	0.2026 (2)	0.4160 (2)	4.04 (7)
C(37)	0.5047 (2)	0.2495 (2)	0.3596 (2)	4.81 (7)
C(38)	0.4965 (2)	0.2260 (2)	0.2780 (2)	4.68 (7)
C(39)	0.4518 (2)	0.1530 (2)	0.2526 (2)	3.98 (6)
C(40)	0.4179 (2)	0.1023 (2)	0.3091 (2)	3.20 (6)
C(41)	0.4603 (2)	-0.0136 (2)	0.1813 (2)	5.40 (8)
C(42)	0.2156 (2)	-0.2065 (2)	0.2232 (2)	4.55 (7)
C(43)	0.2354 (3)	-0.0778 (2)	0.6101 (2)	6.6 (1)
C(44)	0.4881 (2)	0.1107 (2)	0.5757 (2)	4.55 (7)

to 1.00. The space group was determined as *P*2₁/*c* (No. 14) based on the systematic absences. The structure was solved by standard heavy-atom methods. One asymmetric unit contains two [Cu(tmtaa)] molecules. The development of the structure was done by an alternating sequence of least-squares refinements (on *F*) and difference Fourier maps. All non-H atoms were treated anisotropically. All H atoms were located in difference Fourier maps and refined freely. 663 parameters were refined to give *R* = 0.0355 and *wR* = 0.0482; *w* = 1/σ²(*F*_o). The final largest |Δ|σ| = 0.3; the largest peak was 0.2 (1) e Å⁻³; *S* = 1.43. Scattering factors and anomalous-scattering corrections were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Refinement was performed with the Enraf-

Nonius (1979) SDP programs on a DEC MicroVAX II computer. The final positional and equivalent isotropic thermal parameters are listed in Table 1.*

Discussion. ORTEP (Johnson, 1965) drawings of the two independent molecules, including the atom-numbering schemes, are presented in Fig. 1; Fig. 2 shows a side view of one of the molecules (the other being virtually indistinguishable). Important interatomic dimensions for one [Cu(tmtaa)] molecule are presented in Table 2; the other [Cu(tmtaa)] molecule has virtually identical parameters.

* Lists of structure factors, anisotropic thermal parameters and complete intramolecular bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55063 (34 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0609]

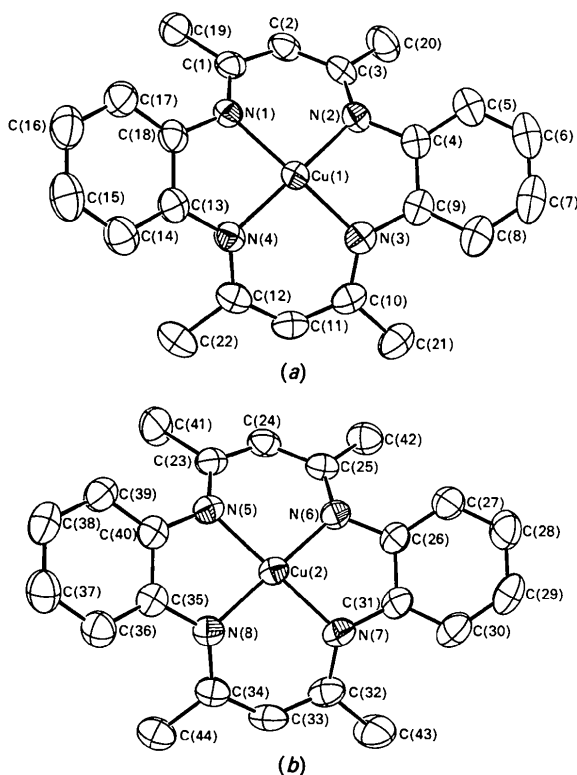


Fig. 1. Views of the two crystallographically independent [Cu(tmtaa)] molecules showing the atomic numbering schemes.

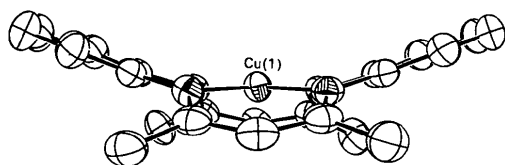


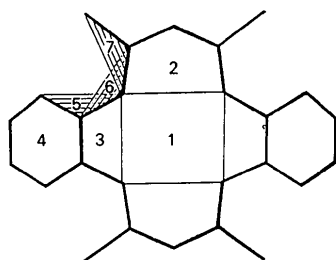
Fig. 2. A side view of one [Cu(tmtaa)] molecule.

Table 2. Selected bond distances (Å) and bond angles (°) for [Cu(tmtaa)]

Numbers in parentheses are e.s.d.'s in the least significant digits.			
Cu(1)—N(1)	1.948 (2)	N(3)—C(10)	1.329 (4)
Cu(1)—N(2)	1.929 (2)	N(4)—C(12)	1.325 (3)
Cu(1)—N(3)	1.935 (2)	N(4)—C(13)	1.413 (3)
Cu(1)—N(4)	1.925 (2)	N(5)—C(23)	1.325 (4)
Cu(2)—N(5)	1.924 (2)	N(6)—C(25)	1.326 (4)
Cu(2)—N(6)	1.927 (2)	N(6)—C(26)	1.409 (4)
Cu(2)—N(7)	1.929 (2)	N(7)—C(31)	1.406 (3)
Cu(2)—N(8)	1.922 (2)	N(7)—C(32)	1.332 (3)
N(1)—C(1)	1.323 (4)	N(8)—C(34)	1.334 (3)
N(1)—C(18)	1.409 (4)	N(8)—C(35)	1.415 (4)
N(2)—C(3)	1.331 (4)	C(4)—C(9)	1.409 (4)
N(2)—C(4)	1.414 (4)	C(13)—C(18)	1.425 (4)
N(3)—C(9)	1.410 (4)	C(26)—C(31)	1.417 (4)
N(1)—Cu(1)—N(2)	95.06 (9)	C(9)—N(3)—C(10)	126.7 (2)
N(1)—Cu(1)—N(3)	176.50 (9)	Cu(1)—N(4)—C(12)	121.8 (2)
N(1)—Cu(1)—N(4)	84.38 (9)	Cu(1)—N(4)—C(13)	111.2 (2)
N(2)—Cu(1)—N(3)	84.2 (1)	C(12)—N(4)—C(13)	126.1 (2)
N(2)—Cu(1)—N(4)	175.17 (9)	Cu(2)—N(5)—C(23)	121.9 (2)
N(3)—Cu(1)—N(4)	96.0 (1)	Cu(2)—N(6)—C(25)	122.9 (2)
N(5)—Cu(2)—N(6)	95.33 (9)	Cu(2)—N(6)—C(26)	110.7 (2)
N(5)—Cu(2)—N(7)	177.09 (9)	C(25)—N(6)—C(26)	125.9 (2)
N(5)—Cu(2)—N(8)	84.75 (9)	Cu(2)—N(7)—C(31)	110.6 (2)
N(6)—Cu(2)—N(7)	83.96 (9)	Cu(2)—N(7)—C(32)	121.7 (2)
N(6)—Cu(2)—N(8)	174.46 (9)	C(31)—N(7)—C(32)	126.9 (3)
N(7)—Cu(2)—N(8)	95.69 (9)	Cu(2)—N(8)—C(34)	122.1 (2)
Cu(1)—N(1)—C(1)	122.0 (2)	Cu(2)—N(8)—C(35)	111.1 (2)
Cu(1)—N(1)—C(18)	110.7 (2)	C(34)—N(8)—C(35)	125.7 (2)
C(1)—N(1)—C(18)	126.1 (2)	N(2)—C(4)—C(9)	114.8 (3)
Cu(1)—N(2)—C(3)	121.7 (2)	N(3)—C(9)—C(4)	114.7 (2)
Cu(1)—N(2)—C(4)	110.8 (2)	N(4)—C(13)—C(18)	114.7 (2)
C(3)—N(2)—C(4)	126.0 (3)	N(1)—C(18)—C(13)	114.5 (2)
Cu(1)—N(3)—C(9)	110.7 (2)	N(6)—C(26)—C(31)	114.3 (2)
Cu(1)—N(3)—C(10)	121.9 (2)	N(7)—C(31)—C(26)	114.4 (3)

As seen in Figs. 1 and 2, the general shape of the [Cu(tmtaa)] molecule resembles that of [Fe(tmtaa)] (Goedkin, Pluth, Peng & Bursten, 1976) and several others of the general formula [M(tmtaa)]X, the structures of which have been previously reported (Weiss, Bursten, Peng & Goedkin, 1976). The Cu^{II} ion is clearly four-coordinate with an average Cu—N distance of 1.930 (2) Å. The latter can be compared with the similar distances of 1.930–1.939 Å found in the [Cu(phthalocyanine)] complex (Brown, 1968). However, this Cu—N_{av} distance is much shorter than the corresponding metal—N distance of 1.996 (5) Å observed in [Pd(tmtaa)] (Tsutsui, Bodsein, Cash & Pettersen, 1979). This comes as no surprise since the ionic radius of Cu²⁺ (0.76 Å) is much smaller than that of Pd²⁺ (0.86 Å) (Shannon, 1976).

A noteworthy feature of the [Cu(tmtaa)] structure is the small displacement (0.070 Å) of the Cu atom from the plane of the four N atoms towards the side of the ligand to which the benzenoid rings are tipped. The displacement is smaller than that in the [Fe(tmtaa)] complex, where the Fe center is 0.114 Å from the plane. Two factors contribute to this difference: (1) a stronger preference of copper(II) over that of iron(II) for square coordination; (2) the ionic radius of Cu²⁺ which is 0.04 Å smaller than that of Fe²⁺ (Shannon, 1976). Nevertheless, these two factors are not enough to force the ligand to adopt a step-like geometry. Instead, in [Cu(tmtaa)]

Table 3. Comparison of selected dihedral angles ($^{\circ}$) for $M(\text{tmtaa})$ compounds

Planes	H_2tmtaa	$[\text{Fe}(\text{tmtaa})]$	$[\text{Pd}(\text{tmtaa})]$	$[\text{Cu}(\text{tmtaa})]$
1-2	34.3	24.5	14.7	26.0
1-3	20.1	17.5	1.4	16.2
1-4	24.6	23.7	13.0	21.0
5-6	45.6	31.5	25.0	34.1
6-7	3.6	9.27	5.2	5

the metal center comes as close as it can to achieving a square-planar coordination with tmtaa without forcing the centrosymmetric geometry upon the ligand.

Although only a handful of $[M(\text{tmtaa})]$ -type complexes have been structurally characterized to date, it is worthwhile to compare some of their features. Table 3 presents the dihedral angles for these compounds. These dihedral angles are good indicators of the degree of deviation of the macrocyclic ligand from planarity. The free ligand as well as the ligands in the complexes with iron and copper have similar saddle-shape conformations. For $[\text{Pd}(\text{tmtaa})]$, on the

other hand, deviations from planarity are much smaller. Table 3 also shows that the shapes of the $[\text{Cu}(\text{tmtaa})]$ and $[\text{Fe}(\text{tmtaa})]$ molecules are very similar, despite a smaller displacement of the Cu center out of the N_4 plane.

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Structure of 3,5-Dimethyl-1,2-tellurazole

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Abstract. 3,5-Dimethyl-1,2-tellurazole, $\text{C}_5\text{H}_7\text{NTe}$, $M_r = 208.7$, monoclinic, $P2_1/c$, $a = 13.592$ (3), $b = 11.460$ (3), $c = 25.751$ (9) Å, $\beta = 101.08$ (2) $^{\circ}$, $V = 3936$ (2) Å 3 , $Z = 24$, $D_x = 2.113$ g cm $^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 44.3$ cm $^{-1}$, $F(000) = 2304$, $T = 298$ K, final $R = 0.045$ and $wR = 0.057$ for 5298 reflections with $I > 3\sigma(I)$. The title compound is monomeric in the gaseous state and in solution, and forms $\text{Te}\cdots\text{N}$ intermolecular bonds in the solid state.

Introduction. Monocyclic derivatives of 1,2-tellurazole were synthesized for the first time in 1983 (Lucchesini & Bertini, 1983) by reacting α -acetylenic

oxime-*O*-sulfonic acids with potassium telluride in aqueous medium. They are rather stable solids, which can be crystallized from the usual organic solvents and from the melt without decomposition. Their melting point is considerably higher than that of the selenium-containing isologues, which are liquid at room temperature (Lucchesini, Bertini & De Munno, 1984); it is also higher than that of the tellurophene analogues (Mack, 1966). Low solubility and high melting point were also found for 1,2,5-telluradiazole, with respect to the selenium homologue (Bertini, Dapporto, Lucchesini, Sega & De Munno, 1984).