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Synthesis and Structure of a Novel Cu(II) Complex with a Monoprotic Tetradentate Schiff Base Ligand

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Introduction

Radiopharmaceuticals labeled with positron-emitting copper radioisotopes have potential for clinical use in diagnostic imaging by positron emission tomography (PET).[1] As part of a continuing investigation of radiocopper complexes,[2−5] we have focused on the synthesis of copper chelating ligands that can be readily derivatized to alter and optimize radiotracer biodistribution and pharmacokinetics. We have recently synthesized a monoprotic tetradentate Schiff base ligand, *N*-(2-pyridylmethyl)-*N′*-(salicyaldimino)-1,3-propanediamine, or Hpaip (Figure 1), designed to possibly afford a lipophilic monocationic Cu(II) radiotracer for heart imaging.[6]

Like other tetradentate Schiff base ligands derived from linear diamine backbones, Hpaip can presumably bind a Cu(II) center in a square-planar manner. Our goal in radiopharmaceutical design with this ligand was to obtain a monocationic Cu(II) complex with a saturated square-planar coordination sphere. To our knowledge there have been no structural reports on Cu(II) complexes with such potentially planar tetradentate monoprotic ligands presenting one oxygen and three nitrogen donor atoms. The only previously reported structurally characterized Cu(II) complex with a tetradentate monoprotic ligand is instead derived from a tripodal tertiary amine bearing two pyridyl arms and one phenolate pendant arm.[7,8] Owing to the nonlinear NN_2O donor set of this tripodal ligand, a square-pyramidal Cu(II) complex was formed with the NN_2 donors from the ligand on the basal plane along with a Cl donor, while the phenolate O was bound in the apical position. Thus, the structure revealed a neutral complex with a regular Cu−Cl bond.

We report here an investigation of Cu(II) coordination chemistry with Hpaip which shows the Cu complex to adopt a square-based pyramidal geometry in the solid state with a weak Cu−Cl bond in the axial site.

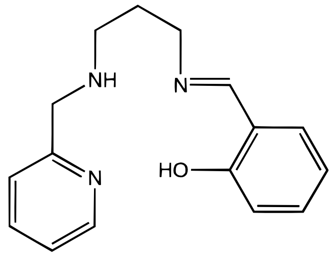

Figure 1. Monoprotic tetradentate Schiff base ligand, Hpaip.

Experimental Section

General. All chemicals were reagent grade and were used as received. FAB-mass spectra were recorded with a Kratos MS50 mass spectrometer (with positive ion detection). Infrared spectra were recorded with a Perkin-Elmer FTIR spectrophotometer and were referenced to polystyrene. Elemental analyses were performed in the Microanalytical Service Lab in the Department of Chemistry, Purdue University.

Hpaip. This was synthesized by modification of a previously described procedure.[6] Briefly, 2-(aminomethyl)pyridine (20.32 g, 0.19 mmol) and acrylonitrile (10.61 g, 0.21 mmol) were mixed and stirred for 2 days. The resultant yellow liquid was heated (70 °C) in vacuo overnight to remove the remaining acrylonitrile. The yield of crude *N*-(2-cyanoethyl)-2′-pyridylmethylamine was 29.92 g (99.8%). The *N*-(2-cyanoethyl)-2′-pyridylmethylamine (6.52 g, 40.4 mmol) was added dropwise to a stirred, pre-prepared suspension of $AlCl_3$ (13.33 g) and 42.0 mL of 1 M $LiAlH_4$ in THF, in 200 mL of Et_2O. The mixture was stirred for 40 h, then it was cooled to 0 °C, and to it was cautiously added 100 mL of 30% KOH in water. The ether layer was collected, and the remaining emulsion was loaded onto 4 Å molecule sieves in a thimble. The solidified emulsion was extracted overnight with $CHCl_3$ using a Soxhlet extractor. The ether and chloroform extractants were combined and concentrated into an oil, which was further dried in vacuo overnight. The yield of the crude *N*-(2-pyridylmethyl)-1,3-propanediamine was 4.93 g (73.8%; brown-red oil). The crude *N*-(2-pyridylmethyl)-1,3-propanediamine (1.12 g, 6.78 mmol) was mixed with salicylaldehyde (0.87 g, 6.98 mmol) in EtOH (5 mL) and stirred overnight. After removal of the solvents, the resultant brown oil was purified on a silica gel column eluted with methanol. The purity of the product was verified by ^{1}H NMR. Yield was 0.15 g (8.2%; overall yield, 6.1%).

[Cu(paip)Cl]. To a solution of Hpaip (0.15 g, 0.56 mmol) in 10 mL of $CHCl_3$ was added $CuCl_2{\cdot}2H_2O$ (88 mg, 0.52 mmol). The resultant green solution was stirred and refluxed for 2 h, during which time a gray-green precipitate was formed from the brownish green solution. The precipitate was isolated by filtration, recrystallized from MeOH−$CHCl_3$ (1:1)/Et_2O, washed with Et_2O (2 × 5 mL), and dried in vacuo. The yield was 0.155 g (73% based on Cu). The product is soluble in MeOH, EtOH, and H_2O, moderately soluble in hot $CHCl_3$ and CH_2Cl_2, but not soluble in Et_2O. Anal. Calcd (found) for $C_{16}H_{18}N_3ClCuO{\cdot}(H_2O)_{0.3}.(CHCl_3)_{0.06}$: C, 50.78 (50.96); H, 4.95 (5.02); N, 11.06 (11.20); Cl 11.01 (10.99). FABMS: $m/z = 331$ ($[Cu(paip)]^+$). IR (cm^{-1}, KBr disk): 3080 (m, aromatic ν_{C-H}); 2885 (m, methylene ν_{C-H}); 1630 (vs).

X-ray Crystallographic Analyses of [Cu(paip)Cl]·$CHCl_3$. Single crystals of [Cu(paip)Cl]·$CHCl_3$ were obtained by slow diffusion of Et_2O into a solution of the sample in MeOH/$CHCl_3$ (1:2).

A green chunk of approximate dimensions 0.25 × 0.17 × 0.16 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were both performed on an Enraf Nonius CAD4 diffractometer equipped with a graphite crystal, incident beam monochromator with Cu Kα radiation ($\lambda = 1.541\,84$ Å) at 296

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°K. The cell constants and an orientation matrix for data collection were obtained from least-squares refinement using the setting angles of 25 reflections in the range $23 < \theta < 46°$.

Data were collected at 296 ± 1 K using variable speed $\omega - 2\theta$ scans with the scan rate varying from 2 to 16° per minute, and a maximum 2θ of 148.7°. A total of 4589 reflections were collected, of which 2559 were unique. Lorentz and polarization corrections were applied to the data. An empirical absorption correction based on the method of Walker and Stuart was also applied.[9] Transmission coefficients ranged from 0.221 to 0.350 with an average value of 0.312.

The complex crystallizes in the monoclinic $Pca2_1$ (No. 29) space group established by the systematic absences: $h0l$ $h = 2n$, $0kl$ $l = 2n$. The orthorhombic cell parameters and calculated volume are $a = 11.837(4)$ Å, $b = 15.648(5)$ Å, $c = 11.002(11)$ Å, $V = 2037(3)$ Å^3. For $Z = 4$ and fw = 486.71 for $C_{17}H_{19}N_3Cl_4OCu$, the calculated density is 1.586 g/cm^3. The structure was solved using the structure solution program PATTY in DIRDIF92.[10] The remaining atoms were located in succeeding difference Fourier syntheses. Hydrogen atoms were located and added to the structure factor calculations, but their positions were not refined. The structure was refined in full-matrix least-squares where the function minimized was $\sum w(|F_o| - |F_c|)^2$ and the weight w is defined as $4F_o^2/\sigma^2(F_o^2)$. Scattering factors were taken from Cromer and Waber.[11] Anomalous dispersion effects were included in F_c;[12] the values for f' and f'' were also taken from Cromer.[13] Only the 1188 reflections having intensities greater than 3.0 times their standard deviations were used in refinements. The final refinement cycle included 234 variable parameters and converged with unweighted and weighted agreement factors of $R = \sum|F_o - F_c|/\Sigma F_o = 0.040$ and $R_w = \mathrm{SQRT}(\sum w(F_o - F_c)^2/\sum wF_o^2) = 0.046$, respectively. Refinement was done using MolEN.[14] The highest peak in the final difference Fourier map had a height of 1.33 e$^-$/A^3 with an estimated error based on δF of 0.18.[15] Plots of $\sum w(|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, $\sin \theta/\lambda$, and various classes of indices showed no unusual trends.

Results and Discussion

Synthesis and Characterization. The novel tetradentate ligand (Hpaip) was prepared following a general procedure described previously[6] but with addition of Soxhlet extraction to improve recovery of the *N*-(2-pyridylmethyl)-1,3-propanediamine intermediate. The reaction of the neutral ligand, Hpaip, and $CuCl_2 \cdot 2H_2O$ in $CHCl_3$ was easily accomplished to give the product [Cu(paip)Cl] in high yield. This is consistent with the high radiochemical purity found in preparing the ^{67}Cu-complex of the ligand.[6] The complex is air stable in the solid state and in solution. The radiocopper analogue has also been found to be stable in vitro over 12 h in both absolute ethanol and 5% ethanol/saline.[6]

Mass spectrometric data (FAB) showed no evidence for the [Cu(paip)Cl] parent ion, instead exhibiting a peak at m/z 331 for the $[Cu(paip)]^+$ fragment after loss of the chloride. The chloride coordination to the Cu(II) center may be relatively weak as suggested by the long Cu−Cl distance in solid state (vide infra). Cellulose acetate electrophoresis studies with ^{67}Cu-labeled [Cu(paip)]Cl in aqueous phosphate buffer (pH 7.5) show the radiolabel to migrate as a single peak toward the cathode. indicating the chloride ligand is at least partially dissociated in solution.[16]

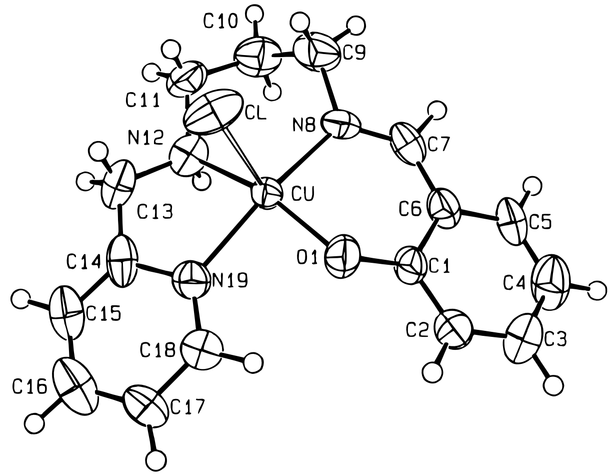

Figure 2. ORTEP drawing of $[Cu(paip)Cl] \cdot CHCl_3$ with the chloroform of solvation omitted; 20% probability thermal ellipsoids are shown.

Table 1. Crystallographic Data for $[Cu(paip)Cl] \cdot CHCl_3$

empirical formula	$CuCl_4ON_3C_{17}H_{19}$
fw	486.71
space group	$Pca2_1$ (No. 29)
a, Å	11.837(4)
b, Å	15.648(5)
c, Å	11.002(11)
V, Å^3	2037(3)
Z	4
d_{calc}, g cm^{-3}	1.586
h, k, l range	0 to 13, 0 to 14, −19 to 19
scan width, deg	$1.22 + 0.24 \tan(\theta)$
F_{000}	988.0
R_{int}	0.035
$R(F_o)$	0.040
$R_w(F_o)$	0.046
goodness of fit	1.251

Table 2. Selected Bond Distances (Å) for $[Cu(paip)Cl] \cdot CHCl_3$[a]

Cu−Cl	2.558(3)	Cu−N12	2.030(6)
Cu−O1	1.909(5)	Cu−N19	2.057(7)
Cu−N8	1.973(7)		

[a] Numbers in parentheses are estimated standard deviations in the least-significant digits.

X-ray Structures of $[Cu(paip)Cl] \cdot CHCl_3$. The copper atom in the [Cu(paip)Cl] complex was found to have a coordination number of 5, with the chloroform of solvation having no direct contact with the copper complex. With the deprotonated tetradentate ligand bound to the Cu(II) center, a neutral complex is formed with a fifth bond to a chloride ligand. An ORTEP diagram of the molecule is shown in Figure 2, while the crystallographic data, selected bond distances, and selected angles are listed in Tables 1, 2, and 3, respectively.

Although 17-electron Cu(II) complexes with four metal-donor bonds are common, five-coordinate Cu(II) complexes with 19 electrons are not unusual.[17] A five-coordinate metal complex can take an intermediate geometry between a regular square pyramid and a regular trigonal bipyramid.[18] The bond angles

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Table 3. Selected Bond Angles (deg) for [Cu(paip)Cl]·CHCl$_3$[a]

Cl−Cu−O1	102.4(2)	O1−Cu−N12	163.5(3)
Cl−Cu−N8	99.5(2)	O1−Cu−N19	88.3(3)
Cl−Cu−N12	91.6(2)	N8−Cu−N12	93.8(3)
Cl−Cu−N19	94.9(2)	N8−Cu−N19	165.0(3)
O1−Cu−N8	92.5(3)	N12−Cu−N19	81.6(3)

[a] Numbers in parentheses are estimated standard deviations in the least-significant digits.

typical of square-pyramidal (2 × 160−170° and 4 × 95−100°) and trigonal-bipyramidal (1 × 180° and 3 × 120°) coordination can both, in a first approximation, describe the coordination geometry in [Cu(paip)Cl]. Based on the deviation from these two models, the coordination geometry of [Cu(paip)Cl] is best described as a distorted square pyramid, with the four donor atoms (NNNO) of the Schiff base ligand on the equatorial plane, the chloro ligand loosely bound on a tilted apical position. The four paip donor atoms (N8, N12, N19, and O1), are nearly coplanar, deviating by 0.0066(75), 0.0063(77), 0.0087(66), and 0.0069(76) Å, respectively, from their least-squares plane. The Cu(II) center is lifted 0.2512(4) Å above this least-squares plane toward the apical chloride ligand (Figure 2).

The distortion from a regular square pyramid is caused in part by the lack of symmetry in the ligand itself. The ligand not only contains four types of binding sites (that differ in charge, hardness, polarizability, and affinity to the copper(II) center) but also forms three unique chelate rings. This, in turn, may play a role in inclining the apical Cu−Cl bond. The distortion of the coordination sphere from a regular square pyramid can be described in both bonding angles and bond distances in the molecule (Tables 2 and 3). For the angular distortion, the apical Cu−Cl bond tilts significantly toward the sector between the Cu−N$_{\text{py}}$ (i.e., Cu−N19), and Cu−N$_{\text{amino}}$ (i.e., Cu−N12) bonds (Figure 2). The Cl−Cu−O and Cl−Cu−N$_{\text{imino}}$ (Cl−Cu−N8) angles are 102.4(2)° and 99.5(2)°, respectively, while Cl−Cu−N$_{\text{py}}$ (or Cl−Cu−N19) and Cl−Cu−N$_{\text{amino}}$ (or Cl−Cu−N12) angles are 94.9(2) and 91.6(2)°, respectively (Table 3). While the large Cl−Cu−O angle can be explained by the repulsion between the negatively charged Cl and phenolate O atoms, the large Cl−Cu−N$_{\text{imino}}$ (Cl−Cu−N8) is probably caused by increased N$_{\text{imino}}$−Cl repulsion due to a shorter Cu−N$_{\text{imino}}$ bond as compared to other two Cu−N bonds (Table 2).

Within the ligand−metal fragment, the four adjacent bond angles about the Cu center are unevenly distributed from the ideal 90°. While the N$_{\text{imino}}$−Cu−O (N8−Cu−O1) and N$_{\text{amino}}$−Cu−N$_{\text{imino}}$ (N12−Cu−N8) bond angles (each of which is within a six-membered ring) are 92.5(3) and 93.8(3)°, respectively, the five-membered chelate-ring-contained N$_{\text{py}}$−Cu−N$_{\text{amino}}$ (N19−Cu−N12) is only 81.6(3)°, and the N$_{\text{py}}$−Cu−O (N19−Cu−O1) of the open sector is 88.3(3)°. Although the angles are unevenly distributed, none of the angles is unusual relative to the chelate rings found in other Schiff base complexes of copper(II). Such N$_{\text{py}}$−Cu−N$_{\text{amino}}$ bond angles in five-membered rings have been discovered in a range of 79−84°,[19,20] while N−Cu−N angles in six-membered propane-based chelate rings have been found in the range of 91 to 97°.[21−23] The N$_{\text{imino}}$−Cu−O angles within the six-membered chelate ring in complexes [Cu(salen)][23] or [Cu(saltn)][24] have been found in the range of 91−93.5°.

In square-pyramidal complexes with an apical Cu−Cl bond, the Cu−Cl distances observed are in the range from 2.39 to 2.63 Å, depending on the nature of the basal ligand(s).[25−31] In the present molecule, a Cu−Cl distance of 2.558 Å is found. This is similar to the Cu−Cl distances known for the other complexes containing monoanionic basal NNNO ligand donor sets derived from bidentate ligands, where apical Cu−Cl distances have been found with the values of 2.5096,[25] 2.558, 2.605,[26] and 2.546 Å[27] (mean = 2.555 Å). The same Cu−Cl distance (2.556 Å) was found in a dinuclear complex containing a basal monoanionic NNNO ligand donor set,[28] while in a complex containing a basal monoanionic dithiadioxime (S$_2$N$_2$) ligand, Cu−Cl distance is 2.3931 Å.[29] With a neutral basal (NNNO) ligand, the apical Cu−Cl distance was found to be shorter (2.474 Å),[30] as compared to the Cu−Cl distances in Cu(II) complexes containing monoanionic basal (NNNO) ligands. With a dianionic (N$_2$O$_2$) ligand, a longer Cu−Cl distance of 2.630 Å was observed in the axial site.[31]

The distances of the planar bonds (O$_{\text{ph}}$−Cu, N$_{\text{imino}}$−Cu, N$_{\text{amino}}$−Cu, and N$_{\text{py}}$−Cu) in [Cu(paip)Cl], are in the range from 1.909 to 2.057 Å (Table 2). In comparison to the corresponding bonds in Cu complexes of tetradentate Schiff bases (bis(salicyaldimine),[23,24,32] or bis(pyridylimine)[21,22]), tridentate Schiff bases (salicyaldiminomethylpyridine),[20] or bidentate pyridylamine ligands,[20,33] the O$_{\text{ph}}$−Cu (O1−Cu), N$_{\text{amino}}$−Cu (N12−Cu), and N$_{\text{py}}$−Cu (N19−Cu) bonds are normal, while N$_{\text{imino}}$−Cu (N8−Cu) is very slightly elongated. In previously characterized compounds the O$_{\text{ph}}$−Cu and N$_{\text{imino}}$−Cu bonds are found in the range of 1.85−1.95 Å, and 1.93 to 1.96 Å, respectively.[23,24] The N$_{\text{amino}}$−Cu, and N$_{\text{py}}$−Cu bonds are usually found in the range between 1.94 and 2.06 Å and 1.98 and 2.05 Å,[7,19−22] respectively, as they are in [Cu(paip)Cl]. The slight increase in N$_{\text{imino}}$−Cu is probably due to expansion of the coordination number to 5 in the [Cu(paip)Cl] complex, as is observed in a Cu(II) complex of 2-hydroxypropane backboned Schiff base.[32]

In conclusion, from a monoanionic tetradentate Schiff base ligand, Hpaip, a five coordinate [Cu$^{\text{II}}$(paip)Cl] complex has been synthesized and structurally characterized. The Hpaip ligand, or its derivatives, may be suitable ligands for formulation of

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neutral Cu(II) radiopharmaceuticals with relatively weak Cu–Cl bonds. Work to develop and evaluate copper radiopharmaceuticals with related ligands remains underway.

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Supporting Information Available: Complete tables of crystallographic data, final atomic coordinates and equivalent isotropic thermal parameters, anisotropic thermal parameters, bond lengths, bond angles, torsion angles and intermolecular contacts, and least-squares planes (11 pages). Ordering information is given on any current masthead page.

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