[Electronic Supplementary Information (ESI)]

Supplementary Information for:

"A new phosphonate pendant-armed cross-bridged tetraamine chelator accelerates copper(II) binding for radiopharmaceutical applications"

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Materials and physical methods:

Reagents: Cupric chloride dihydrate was obtained from Aldrich Chemical Company. Paraformaldehyde and triethyl phosphite were obtained from Acros Organics. 1,1,1,3,3,3-hexafluoro-2-propanol was purchased from Alfa Aesar. Trace Metal™ Grade Hydrochloric Acid was obtained from Fischer Scientific. Amberlite CG50 was obtained from Sigma.

Solvents: Methanol (MeOH, ACS grade) was obtained from Pharmco Products Inc. Diethyl ether (Et_2O) and toluene ($PhCH_3$, ACS grade) were obtained from EMD Chemicals Inc. The solvents were stored in an Innovative Technology Inc. Pure-Solv Solvent Purification System. Prior to use, each solvent was passed through the system's alumina column under low pressure to remove trace impurities.

Melting points (mp) were obtained on a Thomas Hoover capillary melting point apparatus and were uncorrected. Elemental analyses were obtained at Atlantic Microlab Inc., Norcross, GA and Schwartzkopf Microanalytical Laboratory, Woodside, NY. Infrared (IR) spectra were run on a Nicolet MX-1 FT-IR spectrometer and absorptions are reported in wavenumbers (cm^{-1}). High-resolution mass spectra were obtained at the Mass Spectrometry

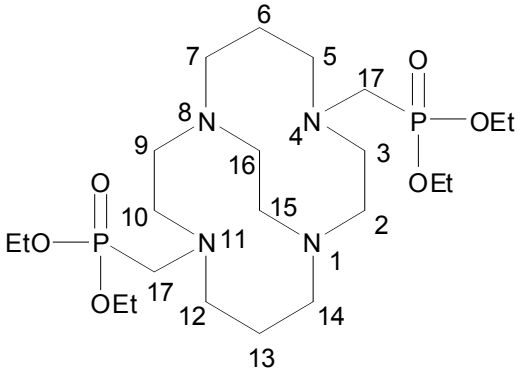
Facility at the University of Notre Dame on a JEOL AX505HA high-resolution mass spectrometer. ^{1}H NMR, ^{13}C{^{1}H} NMR, and ^{31}P{^{1}H} NMR spectra were acquired on a Varian INOVA-500 NMR spectrometer. ^{1}H and ^{13}C chemical shifts are reported in parts per million (ppm) relative to internal Me_4Si (TMS) unless otherwise noted and coupling constants (J) are reported in Hertz (Hz). ^{31}P chemical shifts are reported in parts per million (ppm) relative to an external 85% phosphoric acid standard.

UV-Vis spectra were obtained on a Varian Cary 50 spectrophotometer. Electrochemical studies were performed on a BAS 100B electrochemical analyzer in 0.1 M aq. NaOAc solution using a glassy carbon working electrode, a platinum wire auxiliary electrode, and Ag/AgCl reference electrode. Acid inertness studies were carried out under *pseudo* first-order conditions in 5M HCl solutions at 90° by monitoring the time-dependent decay of the electronic absorption maximum at 630 nm.

Synthesis and characterization of precursor **4** and ligand **2**:

1,4,8,11-tetraazabicyclo[6.6.2]hexadecane-4,11-bis(methanephosphonic acid diethyl ester) (**4**). Triethyl phosphite (0.18 mL, 1.0 mmol) and paraformaldehyde (32.5 mg, 2.5 molar equivalents of CH_2O) were added to a solution of 1,4,8,11-tetraazabicyclo[6.6.2]-hexadecane (**3**) (0.0982 g, 0.4338 mmol) in 1.5 mL of dry THF and stirred under N_2 for 4 days. The solvent was removed, the residue was dissolved in H_2O (20 mL), and the solution was made strongly basic (pH=14, slow addition of KOH pellets). The resulting solution was extracted with toluene (5 x 11 mL), the combined organic phases were dried over anhyd Na_2SO_4, the solvent was removed under aspirator pressure, and the residual solvent was removed under vacuum to give product pure by NMR (0.2156 g, 94%) as a waxy white solid **4**: mp 42-44 ºC; $\nu_{max}(CH_2Cl_2)/cm^{-1}$ 3476, 2980, 2905, 2799, 1669, 1446, 1390, 1366, 1343, 1323, 1292, 1245, 1161, 1126, 1098, 1028; δ_H ($CDCl_3$, 500 MHz, Me_4Si) 1.22-1.32 (14 H, m), 1.32-1.41 (2 H, m), 2.20-2.28 (4 H, m), 2.27-2.35 (2 H, XX´ of AA´XX´, cross-bridge NCH*H*CH*H*N), 2.38 (2 H, dt, *J* 12.0 and 3.2), 2.50-2.75 (6 H, m), 2.60 (2 H, dd, $^{2}J_{HH}$ -15.6, $^{2}J_{HP}$ -2.2, NC*H*HP) 2.77-2.87 (2 H m), 2.82 (2 H, t_{app}, $^{2}J_{HH}$ -16.0, $^{2}J_{HP}$ -16.0, NCH*H*P), 3.04-3.13 (2 H, AA´ of AA´XX´, cross-bridge NCH*H*CH*H*N), 3.70 (2 H, tt, *J* 11.7 and 4.2), 3.99-4.10 (8 H, m, P(O)OCH_2CH$_3$); δ_C ($CDCl_3$, 125.68 MHz, Me_4Si) 15.54 (2 C, d, $^{3}J_{PC}$ 4.8, OCH$_2$*C*H$_3$), 15.59 (2 C, d, $^{3}J_{PC}$ 5.8, OCH$_2$*C*H$_3$), 27.10 ($C_{6,13}$),

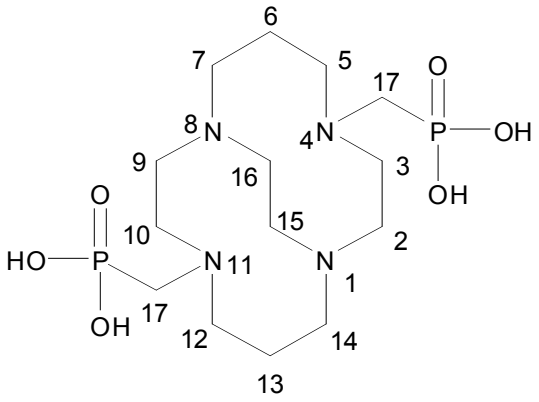
49.24 (2 C, d, $^{1}J_{PC}$ 160.3, N*C*H_2P), 49.88 (coincident with downfield line of doublet at 49.24), 54.94 (2 C, d $^{3}J_{PC}$ 15.4, $C_{5,12}$), 55.55, 55.79 ($C_{15,16}$), 59.41, 60.24 (2 C, d, $^{2}J_{PC}$ 6.7, O*C*H_2CH$_3$), 60.47 (2 C, d, $^{2}J_{PC}$ 7.7, O*C*H_2CH$_3$); [Note: ^{1}H-COSY and gHMQC experiments aided resonance assignments (see structure below for compound numbering)]; δ_P ^{31}P{^{1}H} ($CDCl_3$, 161.83 MHz, external 85% phosphoric acid) 26.98; HRFABMS, *m/z* $(M+H)^+$ exact mass for $C_{22}H_{49}N_4O_6P_2$: 527.3127; Found: 527.3127 (error -0.8 mmu/-1.6 ppm).



Numbering for **4**.

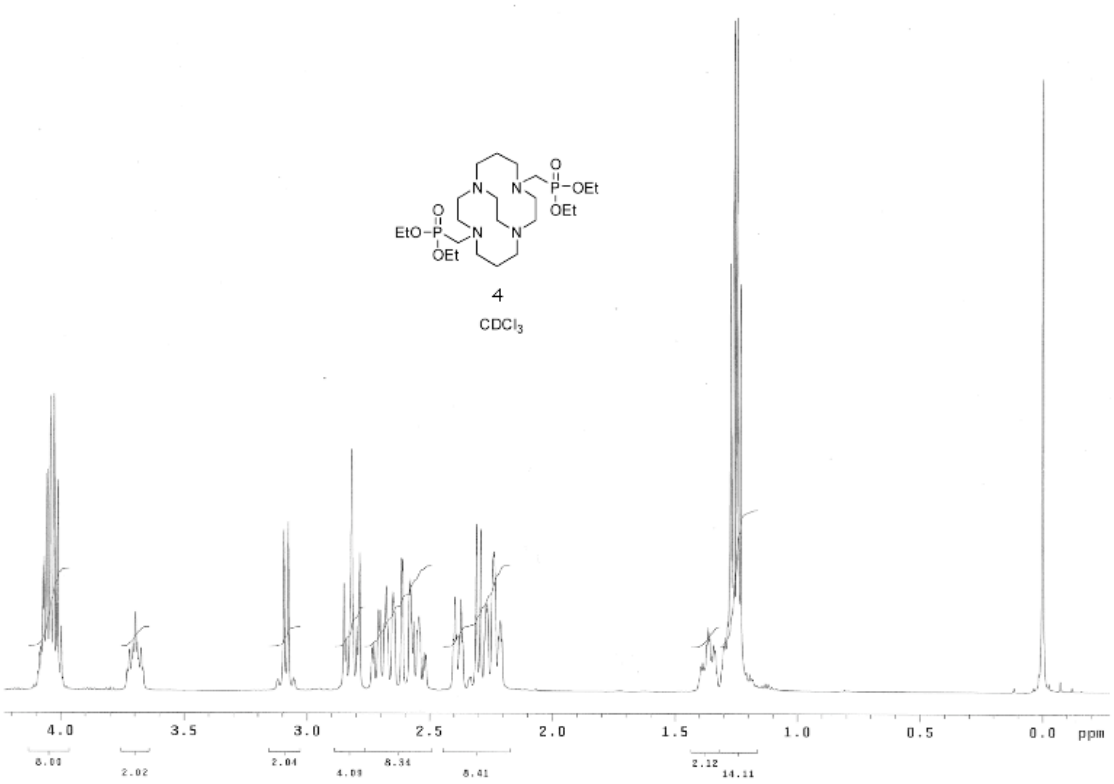
1,4,8,11-Tetraazabicyclo[6.6.2]hexadecane-4,11-bis(methanephosphonic acid) (H_2**2**·0.6HCl·1.1H_2O). 0.3440 g (0.6533 mmol) of **4** was dissolved in 32 mL of 6M HCl and refluxed under N_2 for 1 day. The solvent was removed under reduced pressure and the crude product was dissolved in 4 mL of H_2O and chromatographed using a weakly acidic cation exchange column (Amberlite CG50, H^+ form, 7.7 g, column size = 27 cm x 2 cm). The product was eluted with H_2O (first 30 mL of eluant was discarded), fractions containing the product were combined (35 fractions, 3 mL each), the solvent was removed under reduced pressure, and residual solvent was removed under vacuum to give H_2**2**·0.6HCl·1.1H_2O (0.1919 g, 64%) as a white solid: mp 182-185 ºC (Found: C, 36.56; H, 7.84; N, 12.06; Cl, 4.81. Calc. for $C_{14}H_{32}N_4O_6P_2$·$(HCl)_{0.6}$·$(H_2O)_{1.1}$: C, 36.87; H, 7.69; N 12.28; Cl, 4.66%); ν_{max}(KBr)/cm^{-1} 3397 (br), 2983, 2851, 1655, 1491, 1470, 1241, 1183, 1097, 1073, 1047, 903; δ_H (D_2O, 500 MHz, internal ref C*H*$_3$CN set to 2.06) 1.74-1.83 (2 H, dm, *J* 16.6, H_{6eq}), 2.29-2.42 (2 H, qm-like, H_{6ax}), 2.49-2.58 (2 H, dm, *J* 13.9, H_{2eq}), 2.80-2.93 (4 H, m, $H_{15\ BB'\ of\ AA'BB'}$ and H_7), 2.95-3.18 (8 H, m, $H_{15\ AA'\ of\ AA'BB'}$, H_7, H_{3eq}, NC*H*HP), 3.29-3.37 (2 H, dm, *J* 13.2, H_{5eq}), 3.45 (2 H, td, *J* 13.7 and 3.7, H_{2ax}), 3.76 (2 H, tt_{app}, *J* 14.6 and 3.7, H_{3ax}), 3.96 (2 H, td, *J* 13.0 and 3.4, H_{5ax}), and 4.17 (2 H, t_{app}, , $^{2}J_{HH}$ -14.6, $^{2}J_{PC}$ -14.6, NCH*H*P); δ_C (D_2O, 125.68 MHz, internal *C*H$_3$CN set to 1.47)

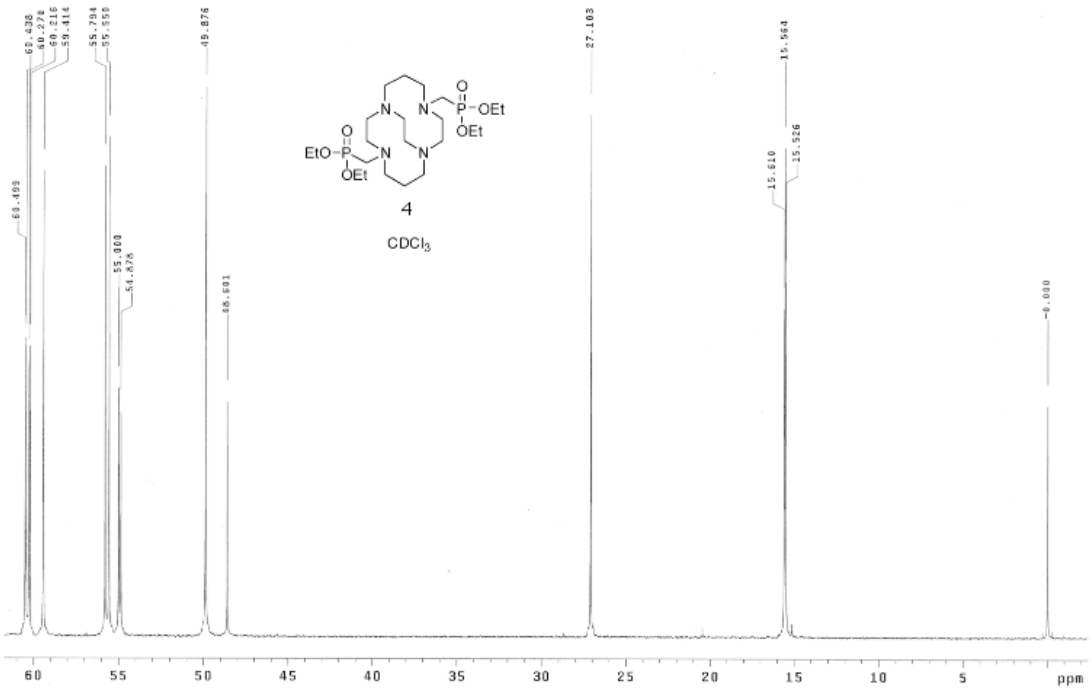
20.23 (C_6), 48.75 (C_{15}), 52.01 (2 C, d, $^1J_{PC}$ 137.2, NCH$_2$P), 52.34 (2 C, d, $^3J_{PC}$ 9.6, C_3), 52.64 (C_2), 58.17 (br, C_5), 58.47 (C_7) [Note: ^{1}H-COSY and gHMQC experiments aided resonance assignments (see structure below for compound numbering)]; δ_P ^{31}P{^{1}H} (D_2O, 161.83 MHz, external 85% phosphoric acid) 9.48 (s); HRFABMS, *m/z* $(M+H)^+$ exact mass for $C_{14}H_{33}N_4O_6P_2$: 415.1875; Found: 415.1877 (error -1.2 mmu/-2.9 ppm). Diffusion of acetone into an aqueous solution of H_2**2**·0.6HCl·1.1H_2O produced crystals suitable for X-ray diffraction.



Numbering for H_2-**2**

1. NMR spectra of precursor **4** and ligand **2**:

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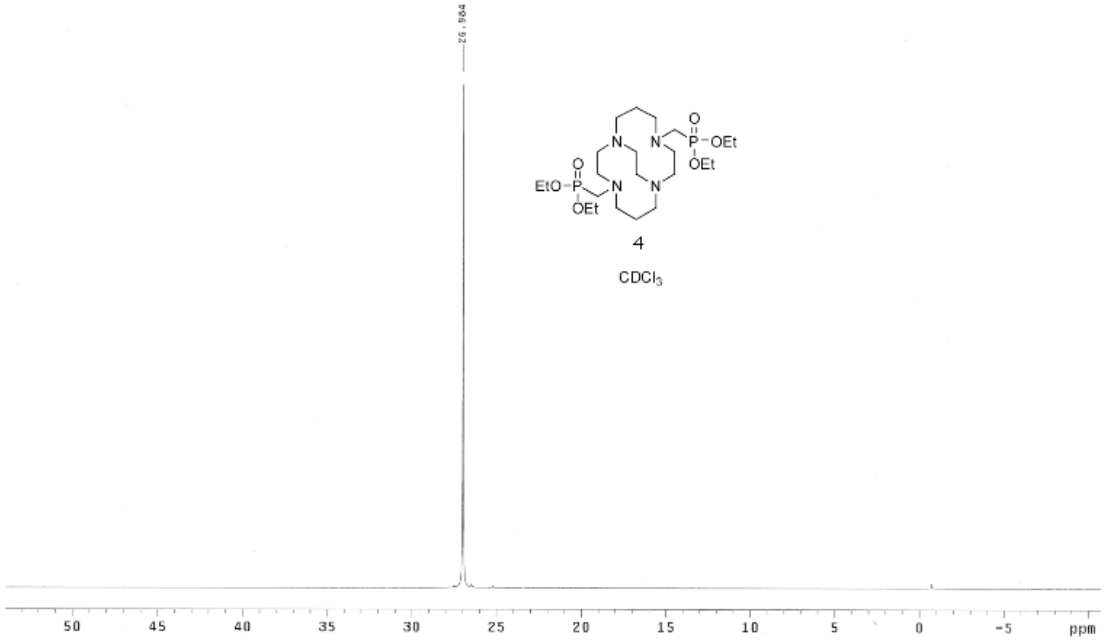
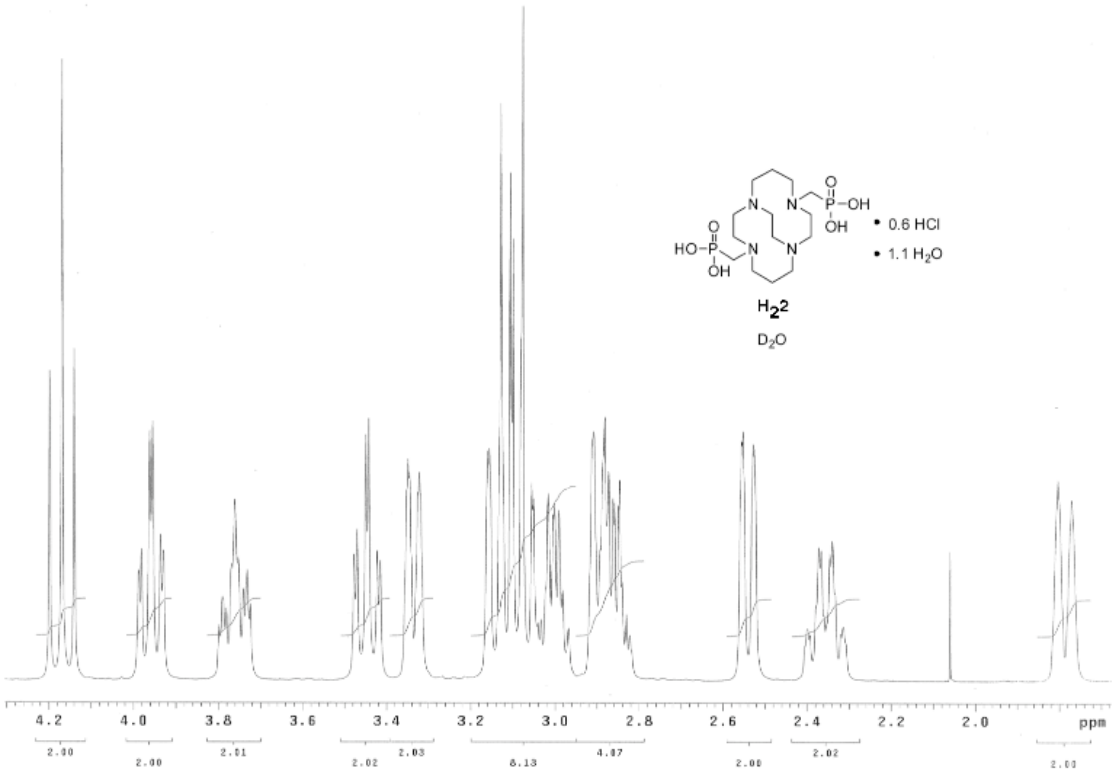
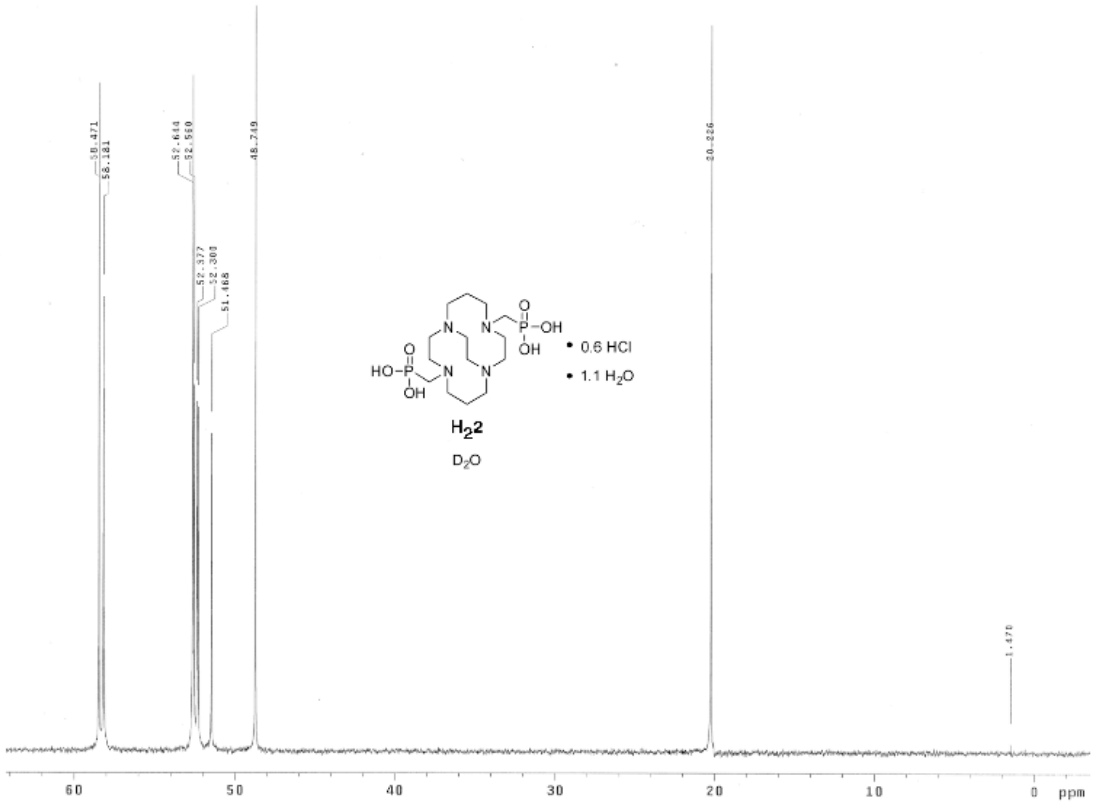
59.414
55.794
55.550
49.876
27.103
15.564
15.526
15.510
60.499
55.000
54.676
48.691
-0.080
4
CDCl3
60
55
50
45
40
35
30
25
20
15
10
5
ppm

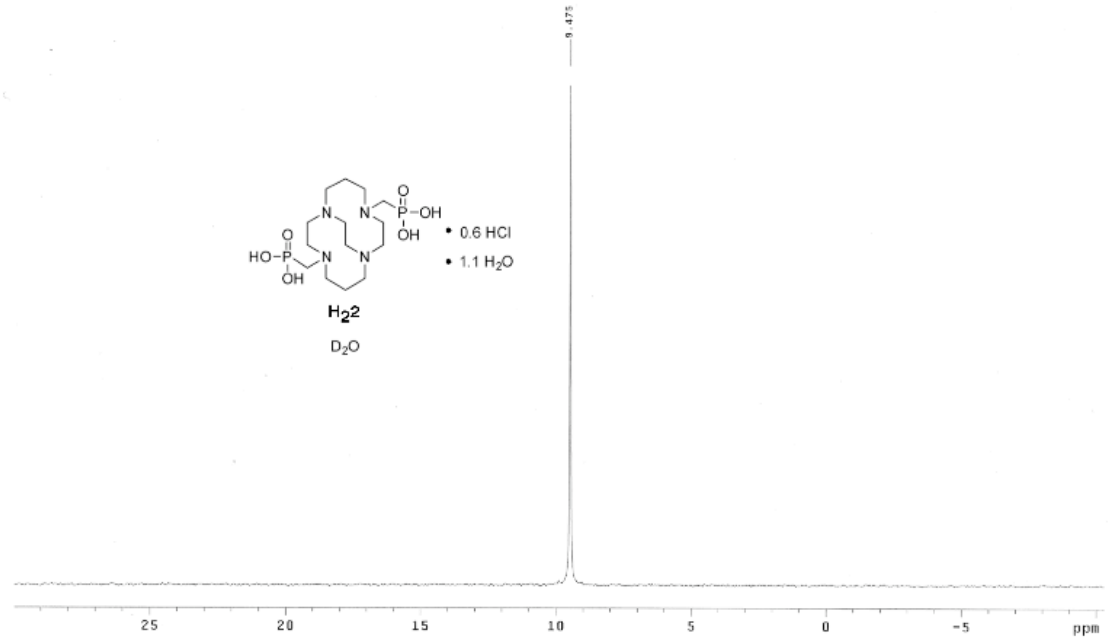


4

$CDCl_3$







Synthesis and characterization of the Cu(II) complex of **2**:

Cu-2: A solution of $CuCl_2 \cdot 2H_2O$ (0.0132 g, 0.077 mmol) in 2 ml MeOH was added to a 2 ml solution of H_2**2**$\cdot 0.6HCl \cdot 1.1H_2O$ (0.035 g, 0.077 mmol) in MeOH. Aq. NaOH (0.3 ml of a 0.4 M solution) was added to raise the *pH* to 5. The resulting blue solution was evaporated to dryness and extracted with 1 ml of 1,1,1,3,3,3-hexafluoro-2-propanol. The NaCl precipitate was separated from the blue supernatant after centrifugation. Diethyl ether diffusion into the supernatant yielded blue microcrystals (0.047 g, 86%) (Found: C 29.48, H 4.96, N 7.91, Cl 1.78, P 8.66. Calc. for $C_{14}H_{30}N_4O_6P_2Cu \cdot H_2O \cdot 0.3NaCl \cdot 1.2C_3H_2F_6O$: C 29.64, H 4.86, N 7.86, Cl 1.49, P 8.69%); UV-Vis: λ_{max} (MeOH)/nm 639 (ε/dm^3 mol^{-1} cm^{-1} 35); HRFABMS (m/z) $C_{14}H_{31}N_4P_2Cu$: calcd 476.1015; found 476.1009 $[M+H]^+$ (error -0.6 mmu/-1.2 ppm). Cyclic voltammogram (0.1M aq. NaOAc): -0.96 V (Ag/AgCl) *quasi*-reversible. X-ray crystals were obtained by diethylether diffusion into a hexafluoro-2-propanol solution of the complex inside a 2-mm inner diameter glass tube.

X-ray crystallography:

X-ray crystallographic data for H_2**2**·HCl·4H_2O:

A colorless crystal of sample Wong151 was mounted on a Cryoloop with Paratone-N oil. Data were collected on a Bruker APEX II CCD systems using Mo K alpha radiation in a stream of nitrogen gas at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 0.5°. Indexing and unit cell refinement indicated a centered, monoclinic lattice. The space group was found to be C2. The Bruker SHELXTL software program and scaled using the SADABS software program. Solution by direct methods (SHELXS) and all non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms except those on O and N atoms were placed on their appropriate parent atom using a riding model. The oxygen atoms on O and N were found from a Fourier difference map, fixed at distances and angles using DFIX and DANG restraints and were allowed to refine. The hydrogen atom on O2 was set to half occupancy. Refinement indicated an enantiomeric mixture with roughly 31.9/68.1 % ratio of isomers.

Table 1. Crystal data and structure refinement for WONG151.

Identification code	wong151	
Empirical formula	C14 H41 Cl N4 O10 P2	
Formula weight	522.90	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2	
Unit cell dimensions	a = 11.5219(16) Å	α= 90°.
	b = 11.7468(16) Å	β= 115.254(3)°.
	c = 9.6554(13) Å	γ = 90°.
Volume	1181.9(3) $Å^3$	
Z	2	
Density (calculated)	1.469 Mg/m^3	
Absorption coefficient	0.353 mm^{-1}	
F(000)	560	
Crystal size	0.20 x 0.20 x 0.05 mm^3	
Crystal color / habit	colorless / block	
Theta range for data collection	2.33 to 28.20°.	
Index ranges	-14<=h<=15, -14<=k<=15, -12<=l<=12	
Reflections collected	6044	
Independent reflections	2590 [R(int) = 0.0271]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	multi-scan/sadabs	
Max. and min. transmission	0.9826 and 0.9327	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2590 / 7 / 167
Goodness-of-fit on F^2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0333, wR2 = 0.0805
R indices (all data)	R1 = 0.0358, wR2 = 0.0817
Absolute structure parameter	0.32(7)
Largest diff. peak and hole	0.511 and -0.207 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for WONG151. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8166(2)	-307(2)	7959(2)	17(1)
C(2)	8345(2)	1304(2)	6344(2)	19(1)
C(3)	9089(2)	2396(2)	6476(3)	21(1)
C(4)	10522(2)	2279(2)	7530(2)	20(1)
C(5)	12104(2)	1750(2)	10021(2)	19(1)
C(6)	12515(2)	1632(2)	11736(2)	20(1)
C(7)	10577(2)	3281(2)	9788(2)	20(1)
N(1)	8410(2)	943(2)	7880(2)	17(1)
N(2)	10783(2)	2178(2)	9168(2)	17(1)
O(1)	8744(2)	-1681(2)	6035(2)	23(1)
O(2)	9340(2)	-2321(1)	8624(2)	20(1)
O(3)	10563(1)	-625(1)	8222(2)	20(1)
P(1)	9324(1)	-1250(1)	7708(1)	16(1)
Cl(1)	10000	5000(1)	5000	24(1)
O(4)	8971(2)	5465(1)	7451(2)	26(1)
O(5)	6660(2)	4509(2)	6283(2)	31(1)

Table 3. Bond lengths [Å] and angles [°] for WONG151.

C(1)-N(1)	1.503(3)	C(2)-C(3)	1.518(3)
C(1)-P(1)	1.828(2)	C(3)-C(4)	1.532(3)
C(2)-N(1)	1.513(3)	C(4)-N(2)	1.483(3)

C(5)-N(2)	1.475(3)	N(1)-C(6)#1	1.506(3)
C(5)-C(6)	1.522(3)	O(1)-P(1)	1.5467(16)
C(6)-N(1)#1	1.506(3)	O(2)-P(1)	1.5334(15)
C(7)-N(2)	1.488(3)	O(3)-P(1)	1.4909(16)
C(7)-C(7)#1	1.550(4)		

N(1)-C(1)-P(1)	115.00(15)
N(1)-C(2)-C(3)	111.38(17)
C(2)-C(3)-C(4)	112.94(18)
N(2)-C(4)-C(3)	112.71(19)
N(2)-C(5)-C(6)	114.03(17)
N(1)#1-C(6)-C(5)	113.11(16)
N(2)-C(7)-C(7)#1	114.11(12)
C(1)-N(1)-C(6)#1	110.17(17)
C(1)-N(1)-C(2)	113.05(16)
C(6)#1-N(1)-C(2)	110.29(16)
C(5)-N(2)-C(4)	108.31(16)
C(5)-N(2)-C(7)	112.04(15)
C(4)-N(2)-C(7)	111.39(16)
O(3)-P(1)-O(2)	116.02(9)
O(3)-P(1)-O(1)	115.75(9)
O(2)-P(1)-O(1)	103.16(9)
O(3)-P(1)-C(1)	107.85(9)
O(2)-P(1)-C(1)	104.53(9)
O(1)-P(1)-C(1)	108.82(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for WONG151. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	14(1)	19(1)	0(1)	9(1)	-1(1)
C(2)	22(1)	19(1)	14(1)	1(1)	5(1)	0(1)
C(3)	21(1)	21(1)	18(1)	3(1)	7(1)	-1(1)
C(4)	21(1)	22(1)	18(1)	2(1)	8(1)	-4(1)
C(5)	16(1)	20(1)	21(1)	3(1)	9(1)	1(1)
C(6)	14(1)	21(1)	22(1)	1(1)	5(1)	-3(1)
C(7)	20(1)	15(1)	22(1)	0(1)	8(1)	-2(1)
N(1)	16(1)	17(1)	16(1)	0(1)	6(1)	-2(1)
N(2)	16(1)	17(1)	18(1)	1(1)	7(1)	1(1)
O(1)	27(1)	22(1)	18(1)	0(1)	8(1)	-2(1)
O(2)	22(1)	18(1)	18(1)	0(1)	7(1)	-1(1)
O(3)	18(1)	22(1)	20(1)	-1(1)	8(1)	-2(1)
P(1)	17(1)	16(1)	16(1)	-1(1)	7(1)	-1(1)
Cl(1)	20(1)	27(1)	22(1)	0	7(1)	0
O(4)	31(1)	21(1)	27(1)	-3(1)	13(1)	-1(1)
O(5)	30(1)	43(1)	25(1)	-10(1)	16(1)	-11(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for WONG151.

	x	y	z	U(eq)
H(1A)	7299	-487	7160	20
H(1B)	8166	-471	8965	20
H(2A)	7438	1419	5614	23
H(2B)	8703	692	5936	23
H(3A)	8722	3007	6874	25
H(3B)	8987	2626	5444	25
H(4A)	10862	1597	7225	24
H(4B)	10982	2952	7396	24
H(5A)	12703	2275	9851	23
H(5B)	12175	997	9602	23
H(6A)	13370	1265	12205	24
H(6B)	12598	2400	12190	24
H(7A)	10442	3883	9017	23
H(7B)	11364	3475	10712	23
H(2O)	9857	-2229	9545	29
H(1N)	9220(30)	1150(20)	8580(30)	23(7)
H(1O)	8720(30)	-1230(30)	5410(30)	34(8)
H(4SA)	9100(40)	6100(20)	7810(40)	61(11)
H(4SB)	9260(20)	5390(20)	6810(30)	24(7)
H(5SA)	6260(30)	4400(40)	6810(40)	64(12)
H(5SB)	7401(18)	4750(20)	6850(30)	30(8)

Table 6. Hydrogen bonds for WONG151 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...N(2)	0.92(3)	2.04(3)	2.868(3)	149(2)
O(4)-H(4SB)...Cl(1)	0.823(17)	2.294(17)	3.1142(19)	175(3)
O(5)-H(5SB)...O(4)	0.842(16)	1.848(18)	2.657(3)	160(3)
O(2)-H(2O)...O(2)#1	0.84	1.61	2.434(3)	165.6
N(1)-H(1N)...N(2)#1	0.92(3)	2.49(3)	2.973(2)	113.3(19)
O(1)-H(1O)...O(5)#2	0.79(3)	1.74(3)	2.508(2)	164(3)
O(4)-H(4SA)...O(2)#3	0.814(18)	1.981(18)	2.795(2)	178(4)
O(5)-H(5SA)...O(3)#4	0.823(18)	1.86(2)	2.673(2)	169(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+2 #2 -x+3/2,y-1/2,-z+1 #3 x,y+1,z

#4 x-1/2,y+1/2,z

X-ray crystallographic data for Cu-**2**:

A crystal was mounted on a Cryoloop with Paratone-N oil and cooled to -173 ^{o}C under a stream of dry nitrogen gas. Data was collected on a BRUKER APEX2 CCD X-ray system using Cu K alpha radiation at -173 ^{o}C and integrated using APEX2 software (SHELXL) corrected for adsorption using SADABS. Structure was solved by direct methods and all non-hydrogen atoms were refined as being anisotropic. Two molecules were found in the asymmetric unit. One of the molecules was disordered and this was treated by assuming a two-position disorder model. Although all the hydrogen atoms were not found, they were included in the chemical formula to account for F000, density and molecular weight.

Disorder associated with Cu-**2** was treated by using a 50% occupancy model for atoms C15, C16, C17, C18, C23, C24, C25, C26, C27, N5, N6, O7, O8, O9, P3, O2SA, O2SB, O6SA, O6SB, C15', C16' C17', C18', C23', C24', C25', C26' C27', N5', N6', O7' , O8', O9', P3' and their associated hydrogen atoms. Occupancy were set for the following atoms at values indicated: Atoms O5SA 40%, O5SB 60%, O7SA and O7SB both at 30 % occupancy while O7SC was at 40% occupancy; atoms Na1A and Na1B 75% and 25% , respectively. The hydrogen atoms on O8 and O8' were fixed in position with appropriate riding models.

Table 1. Crystal data and structure refinement for wong188.

Identification code	wong188
Empirical formula	C14 H34 Cl0.50 Cu N4 Na0.50 O9.50 P2
Formula weight	565.15
Temperature	100(2) K

Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.5428(5) Å	α= 80.039(4)°
	b = 15.5173(7) Å	β= 81.081(4)°
	c = 16.9240(10) Å	γ = 89.874(3)°
Volume	2437.7(2) $Å^3$	
Z	4	
Density (calculated)	1.540 g/cm^3	
Absorption coefficient	3.574 mm^{-1}	
F(000)	1180	
Crystal size	0.31 x 0.21 x 0.05 mm^3	
Theta range for data collection	4.28 to 59.37°	
Index ranges	-10<=h<=10, -17<=k<=17, -16<=l<=18	
Reflections collected	16637	
Independent reflections	6611 [R(int) = 0.0970]	
Completeness to theta = 59.37°	92.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6611 / 0 / 593	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0741, wR2 = 0.1968	
R indices (all data)	R1 = 0.1213, wR2 = 0.2186	
Largest diff. peak and hole	0.941 and -0.730 e $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for wong188. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	3532(1)	5392(1)	7971(1)	17(1)
Cu(2)	-1561(1)	355(1)	8003(1)	19(1)
P(1)	3160(2)	6600(2)	9180(2)	36(1)
P(2)	2181(2)	3816(2)	9406(2)	31(1)
P(3)	-2655(8)	1456(7)	9369(7)	14(3)
P(3')	-3043(9)	1047(9)	9731(8)	23(3)
P(4)	-1868(2)	-1372(2)	9117(2)	36(1)
Na(1)	6652(5)	3467(2)	5571(2)	51(1)
Cl(1)	-3171(2)	-1137(1)	5152(2)	39(1)
O(1)	4074(7)	7460(5)	9046(5)	69(3)
O(2)	2436(6)	6444(4)	10060(4)	46(2)
O(3)	4052(5)	5870(4)	8908(4)	30(2)
O(4)	1754(6)	2949(4)	9120(4)	40(2)
O(5)	1802(6)	3722(4)	10324(4)	43(2)
O(6)	1572(5)	4584(4)	8913(4)	29(2)
O(7)	-3017(11)	1214(8)	10318(8)	20(4)
O(7')	-3246(12)	613(9)	10631(8)	21(4)
O(8)	-3072(11)	2435(7)	9105(8)	16(4)
O(8')	-3665(13)	1937(7)	9648(8)	29(5)
O(9)	-3452(7)	699(7)	9026(6)	91(4)
O(10)	-958(5)	-549(3)	8861(3)	26(1)
O(11)	-2514(6)	-1603(5)	10000(4)	54(2)
O(12)	-970(6)	-2171(4)	8870(4)	41(2)
O(13)	-6353(7)	-797(4)	5703(5)	49(2)
O(14)	8024(7)	2082(4)	4598(4)	49(2)
O(15)	3587(10)	2665(6)	5785(5)	92(3)
O(16)	1085(6)	5124(4)	10889(4)	40(2)
O(17)	-873(7)	-2440(4)	5747(4)	48(2)
O(18)	-3893(7)	-632(9)	10949(5)	120(5)
O(19)	-1311(10)	-3706(8)	4832(7)	121(5)
N(1)	2306(7)	6500(4)	7743(5)	25(2)
N(2)	3113(7)	4799(4)	7043(4)	26(2)
N(3)	4649(7)	4300(4)	8303(4)	23(2)

N(4)	5176(6)	6159(4)	7072(4)	24(2)
N(5)	-439(8)	1284(4)	8378(6)	47(3)
N(6)	-2028(9)	1353(4)	7135(6)	47(3)
N(7)	39(7)	-13(5)	7054(4)	32(2)
N(8)	-2820(7)	-623(4)	7726(4)	23(2)
C(1)	1019(9)	6353(5)	7351(7)	38(3)
C(2)	1290(9)	5902(6)	6628(6)	32(2)
C(3)	1668(9)	4953(5)	6825(6)	32(2)
C(5)	4484(9)	3656(5)	7758(6)	32(2)
C(6A)	3222(9)	3855(5)	7349(5)	25(2)
C(6)	6200(8)	4541(6)	8272(6)	33(2)
C(7)	6951(9)	5023(5)	7450(6)	35(2)
C(8)	6638(8)	5991(5)	7259(6)	31(2)
C(9)	4794(8)	7070(5)	7162(6)	31(2)
C(10)	3218(9)	7205(5)	7180(6)	34(2)
C(11)	4941(9)	5973(5)	6279(6)	31(2)
C(12)	4266(9)	5074(5)	6331(5)	31(2)
C(13)	1798(9)	6741(5)	8540(6)	34(2)
C(14)	4084(8)	3943(6)	9172(5)	28(2)
C(15)	-596(15)	2160(6)	7856(11)	106(7)
C(16)	-1982(14)	2153(6)	7509(10)	89(6)
C(17)	-916(13)	1402(8)	6422(8)	75(5)
C(18)	-247(10)	538(8)	6303(6)	55(3)
C(19)	-307(9)	-926(6)	7099(6)	37(2)
C(20)	-1910(9)	-1084(6)	7148(6)	36(2)
C(21)	-4123(8)	-326(5)	7381(6)	27(2)
C(22)	-3879(9)	451(5)	6685(6)	27(2)
C(23)	-3496(10)	1289(5)	6934(7)	41(3)
C(24)	1147(11)	1081(6)	8268(8)	56(4)
C(25)	1843(11)	956(7)	7452(7)	53(3)
C(26)	1496(9)	90(7)	7229(6)	44(3)
C(27)	-935(12)	1248(8)	9281(9)	69(4)
C(28)	-3294(8)	-1207(6)	8516(6)	32(2)

Table 3. Bond lengths [Å] and angles [°] for wong188.

Cu(1)-O(3)	1.991(6)
Cu(1)-N(2)	2.042(7)
Cu(1)-N(3)	2.042(6)
Cu(1)-N(1)	2.092(6)
Cu(1)-N(4)	2.199(7)
Cu(2)-O(10)	1.989(5)
Cu(2)-N(5)	2.041(7)
Cu(2)-N(6)	2.041(8)
Cu(2)-N(8)	2.096(6)
Cu(2)-N(7)	2.188(7)
Cu(2)-O(9)	2.426(7)
P(1)-O(3)	1.507(6)
P(1)-O(2)	1.520(7)
P(1)-O(1)	1.559(6)
P(1)-C(13)	1.806(10)
P(2)-O(6)	1.503(6)
P(2)-O(5)	1.522(7)
P(2)-O(4)	1.579(6)
P(2)-C(14)	1.801(8)
P(3)-P(3')	0.844(6)
P(3)-O(8')	1.300(12)
P(3)-O(7)	1.568(19)
P(3)-O(8)	1.576(15)
P(3)-O(9)	1.634(11)
P(3)-C(27)	1.660(11)
P(3')-O(7)	1.071(13)
P(3')-O(8')	1.494(15)
P(3')-O(9)	1.496(9)
P(3')-O(7')	1.54(2)
P(3')-C(27)	2.042(17)
P(3')-O(8)	2.23(2)
P(4)-O(10)	1.506(6)
P(4)-O(11)	1.506(7)
P(4)-O(12)	1.585(6)
P(4)-C(28)	1.815(8)
O(7)-O(7')	0.997(13)

O(7)-O(8')	1.643(17)
O(8)-O(8')	1.166(14)
N(1)-C(13)	1.471(11)
N(1)-C(10)	1.499(10)
N(1)-C(1)	1.520(11)
N(2)-C(6A)	1.476(10)
N(2)-C(3)	1.490(10)
N(2)-C(12)	1.502(11)
N(3)-C(14)	1.495(11)
N(3)-C(5)	1.496(11)
N(3)-C(6)	1.518(10)
N(4)-C(11)	1.469(11)
N(4)-C(9)	1.487(10)
N(4)-C(8)	1.490(10)
N(5)-C(15)	1.509(13)
N(5)-C(27)	1.518(16)
N(5)-C(24)	1.535(13)
N(6)-C(17)	1.469(16)
N(6)-C(16)	1.492(13)
N(6)-C(23)	1.500(11)
N(7)-C(19)	1.441(11)
N(7)-C(18)	1.467(12)
N(7)-C(26)	1.480(11)
N(8)-C(20)	1.483(11)
N(8)-C(28)	1.486(11)
N(8)-C(21)	1.493(10)
C(1)-C(2)	1.500(13)
C(2)-C(3)	1.508(12)
C(5)-C(6A)	1.486(12)
C(6)-C(7)	1.530(13)
C(7)-C(8)	1.520(12)
C(9)-C(10)	1.514(12)
C(11)-C(12)	1.521(12)
C(15)-C(16)	1.529(14)
C(17)-C(18)	1.516(17)
C(19)-C(20)	1.537(12)
C(21)-C(22)	1.523(12)
C(22)-C(23)	1.497(12)

C(24)-C(25)	1.481(16)
C(25)-C(26)	1.507(15)

O(3)-Cu(1)-N(2)	174.4(2)
O(3)-Cu(1)-N(3)	88.9(3)
N(2)-Cu(1)-N(3)	85.5(3)
O(3)-Cu(1)-N(1)	87.4(3)
N(2)-Cu(1)-N(1)	98.2(3)
N(3)-Cu(1)-N(1)	174.8(3)
O(3)-Cu(1)-N(4)	94.6(3)
N(2)-Cu(1)-N(4)	86.2(3)
N(3)-Cu(1)-N(4)	99.7(2)
N(1)-Cu(1)-N(4)	84.4(2)
O(10)-Cu(2)-N(5)	89.7(3)
O(10)-Cu(2)-N(6)	174.7(3)
N(5)-Cu(2)-N(6)	85.3(3)
O(10)-Cu(2)-N(8)	87.5(2)
N(5)-Cu(2)-N(8)	174.7(3)
N(6)-Cu(2)-N(8)	97.5(3)
O(10)-Cu(2)-N(7)	92.8(3)
N(5)-Cu(2)-N(7)	100.1(3)
N(6)-Cu(2)-N(7)	86.4(3)
N(8)-Cu(2)-N(7)	84.5(3)
O(10)-Cu(2)-O(9)	87.7(3)
N(5)-Cu(2)-O(9)	83.8(3)
N(6)-Cu(2)-O(9)	93.4(4)
N(8)-Cu(2)-O(9)	91.5(3)
N(7)-Cu(2)-O(9)	176.0(3)
O(3)-P(1)-O(2)	116.5(4)
O(3)-P(1)-O(1)	110.4(3)
O(2)-P(1)-O(1)	106.8(4)
O(3)-P(1)-C(13)	105.1(4)
O(2)-P(1)-C(13)	108.0(4)
O(1)-P(1)-C(13)	109.9(5)
O(6)-P(2)-O(5)	116.3(4)
O(6)-P(2)-O(4)	109.0(3)
O(5)-P(2)-O(4)	110.1(4)
O(6)-P(2)-C(14)	107.1(3)

O(5)-P(2)-C(14)	106.5(4)
O(4)-P(2)-C(14)	107.5(4)
P(3')-P(3)-O(8')	85.6(12)
P(3')-P(3)-O(7)	40.1(8)
O(8')-P(3)-O(7)	69.2(9)
P(3')-P(3)-O(8)	132.1(9)
O(8')-P(3)-O(8)	46.6(7)
O(7)-P(3)-O(8)	108.3(7)
P(3')-P(3)-O(9)	65.5(8)
O(8')-P(3)-O(9)	105.2(7)
O(7)-P(3)-O(9)	105.2(11)
O(8)-P(3)-O(9)	117.7(6)
P(3')-P(3)-C(27)	104.5(9)
O(8')-P(3)-C(27)	146.2(8)
O(7)-P(3)-C(27)	97.8(7)
O(8)-P(3)-C(27)	117.0(11)
O(9)-P(3)-C(27)	108.4(5)
P(3)-P(3')-O(7)	109.4(15)
P(3)-P(3')-O(8')	60.1(10)
O(7)-P(3')-O(8')	77.7(9)
P(3)-P(3')-O(9)	83.6(10)
O(7)-P(3')-O(9)	164.5(16)
O(8')-P(3')-O(9)	102.9(8)
P(3)-P(3')-O(7')	147.2(10)
O(7)-P(3')-O(7')	40.1(9)
O(8')-P(3')-O(7')	110.0(9)
O(9)-P(3')-O(7')	128.6(12)
P(3)-P(3')-C(27)	51.9(7)
O(7)-P(3')-C(27)	97.9(9)
O(8')-P(3')-C(27)	105.5(11)
O(9)-P(3')-C(27)	96.8(7)
O(7')-P(3')-C(27)	110.4(6)
P(3)-P(3')-O(8)	31.6(6)
O(7)-P(3')-O(8)	94.4(11)
O(8')-P(3')-O(8)	28.6(7)
O(9)-P(3')-O(8)	92.8(8)
O(7')-P(3')-O(8)	133.1(7)
C(27)-P(3')-O(8)	80.3(7)

O(10)-P(4)-O(11)	117.4(4)
O(10)-P(4)-O(12)	108.9(3)
O(11)-P(4)-O(12)	108.6(4)
O(10)-P(4)-C(28)	105.0(3)
O(11)-P(4)-C(28)	108.3(4)
O(12)-P(4)-C(28)	108.2(4)
P(1)-O(3)-Cu(1)	116.5(3)
O(7')-O(7)-P(3')	96.0(16)
O(7')-O(7)-P(3)	125.2(14)
P(3')-O(7)-P(3)	30.5(8)
O(7')-O(7)-O(8')	139.1(13)
P(3')-O(7)-O(8')	62.7(10)
P(3)-O(7)-O(8')	47.7(6)
O(7)-O(7')-P(3')	43.9(10)
O(8')-O(8)-P(3)	54.1(8)
O(8')-O(8)-P(3')	37.9(7)
P(3)-O(8)-P(3')	16.3(4)
O(8)-O(8')-P(3)	79.3(12)
O(8)-O(8')-P(3')	113.5(12)
P(3)-O(8')-P(3')	34.3(4)
O(8)-O(8')-O(7)	129.5(11)
P(3)-O(8')-O(7)	63.1(8)
P(3')-O(8')-O(7)	39.6(6)
P(3')-O(9)-P(3)	30.9(3)
P(3')-O(9)-Cu(2)	117.8(5)
P(3)-O(9)-Cu(2)	100.2(5)
P(4)-O(10)-Cu(2)	116.6(3)
C(13)-N(1)-C(10)	112.7(6)
C(13)-N(1)-C(1)	107.9(7)
C(10)-N(1)-C(1)	107.5(7)
C(13)-N(1)-Cu(1)	106.0(5)
C(10)-N(1)-Cu(1)	108.5(5)
C(1)-N(1)-Cu(1)	114.3(5)
C(6A)-N(2)-C(3)	108.1(6)
C(6A)-N(2)-C(12)	109.1(6)
C(3)-N(2)-C(12)	112.4(7)
C(6A)-N(2)-Cu(1)	104.5(5)
C(3)-N(2)-Cu(1)	114.6(5)

C(12)-N(2)-Cu(1)	107.8(5)
C(14)-N(3)-C(5)	112.1(6)
C(14)-N(3)-C(6)	106.4(6)
C(5)-N(3)-C(6)	111.2(7)
C(14)-N(3)-Cu(1)	107.2(5)
C(5)-N(3)-Cu(1)	109.4(5)
C(6)-N(3)-Cu(1)	110.5(5)
C(11)-N(4)-C(9)	111.4(7)
C(11)-N(4)-C(8)	114.8(7)
C(9)-N(4)-C(8)	109.5(6)
C(11)-N(4)-Cu(1)	105.7(5)
C(9)-N(4)-Cu(1)	101.7(5)
C(8)-N(4)-Cu(1)	113.0(5)
C(15)-N(5)-C(27)	114.8(9)
C(15)-N(5)-C(24)	107.2(9)
C(27)-N(5)-C(24)	107.4(8)
C(15)-N(5)-Cu(2)	109.1(6)
C(27)-N(5)-Cu(2)	108.1(7)
C(24)-N(5)-Cu(2)	110.3(5)
C(17)-N(6)-C(16)	110.7(10)
C(17)-N(6)-C(23)	113.0(9)
C(16)-N(6)-C(23)	106.3(8)
C(17)-N(6)-Cu(2)	107.9(6)
C(16)-N(6)-Cu(2)	104.7(7)
C(23)-N(6)-Cu(2)	114.0(6)
C(19)-N(7)-C(18)	113.1(8)
C(19)-N(7)-C(26)	110.2(7)
C(18)-N(7)-C(26)	114.3(7)
C(19)-N(7)-Cu(2)	102.2(5)
C(18)-N(7)-Cu(2)	104.4(6)
C(26)-N(7)-Cu(2)	111.8(6)
C(20)-N(8)-C(28)	111.8(7)
C(20)-N(8)-C(21)	109.2(7)
C(28)-N(8)-C(21)	107.1(6)
C(20)-N(8)-Cu(2)	107.5(5)
C(28)-N(8)-Cu(2)	105.0(5)
C(21)-N(8)-Cu(2)	116.3(5)
C(2)-C(1)-N(1)	115.8(7)

C(1)-C(2)-C(3)	114.2(7)
N(2)-C(3)-C(2)	115.1(7)
C(6A)-C(5)-N(3)	110.6(6)
N(2)-C(6A)-C(5)	112.4(7)
N(3)-C(6)-C(7)	115.3(7)
C(8)-C(7)-C(6)	115.1(7)
N(4)-C(8)-C(7)	113.2(7)
N(4)-C(9)-C(10)	111.4(7)
N(1)-C(10)-C(9)	113.7(7)
N(4)-C(11)-C(12)	113.2(7)
N(2)-C(12)-C(11)	115.5(7)
N(1)-C(13)-P(1)	111.1(6)
N(3)-C(14)-P(2)	115.0(5)
N(5)-C(15)-C(16)	109.2(8)
N(6)-C(16)-C(15)	108.1(9)
N(6)-C(17)-C(18)	115.0(8)
N(7)-C(18)-C(17)	114.2(10)
N(7)-C(19)-C(20)	111.7(7)
N(8)-C(20)-C(19)	114.8(7)
N(8)-C(21)-C(22)	114.4(6)
C(23)-C(22)-C(21)	114.1(8)
C(22)-C(23)-N(6)	116.0(7)
C(25)-C(24)-N(5)	117.9(9)
C(24)-C(25)-C(26)	114.5(8)
N(7)-C(26)-C(25)	115.7(8)
N(5)-C(27)-P(3)	105.4(8)
N(5)-C(27)-P(3')	119.2(7)
P(3)-C(27)-P(3')	23.6(3)
N(8)-C(28)-P(4)	111.0(5)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for wong188. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	20(1)	13(1)	19(1)	-2(1)	-3(1)	2(1)
Cu(2)	21(1)	13(1)	26(1)	-6(1)	-10(1)	4(1)
P(1)	28(1)	38(1)	44(2)	-29(1)	16(1)	-18(1)
P(2)	21(1)	38(1)	32(2)	10(1)	-10(1)	-13(1)
P(3)	16(3)	8(4)	18(5)	-2(4)	-1(3)	-2(3)
P(3')	15(3)	23(6)	32(6)	-8(5)	-5(3)	7(3)
P(4)	17(1)	42(1)	39(2)	18(1)	0(1)	6(1)
Na(1)	80(3)	36(2)	28(3)	7(2)	4(2)	32(2)
Cl(1)	36(1)	41(1)	41(2)	-12(1)	-5(1)	2(1)
O(1)	39(4)	66(5)	104(7)	-66(5)	41(4)	-40(4)
O(2)	35(4)	57(4)	48(5)	-38(4)	15(3)	-19(3)
O(3)	15(3)	43(3)	37(4)	-25(3)	-3(3)	-6(3)
O(4)	35(4)	35(3)	46(5)	13(3)	-20(3)	-17(3)
O(5)	29(3)	71(4)	22(4)	12(3)	-5(3)	-26(3)
O(6)	19(3)	38(3)	23(4)	9(3)	-4(3)	-6(3)
O(7)	31(7)	16(8)	17(9)	-8(6)	-6(6)	-4(5)
O(8)	21(6)	11(7)	13(9)	2(6)	4(5)	2(5)
O(8')	40(8)	19(7)	33(11)	-14(7)	-12(7)	9(6)
O(9)	35(4)	185(9)	101(8)	-129(7)	-42(5)	60(5)
O(10)	13(3)	37(3)	21(4)	7(3)	-1(3)	-6(2)
O(11)	22(3)	78(5)	41(5)	37(4)	6(3)	16(3)
O(12)	27(3)	31(3)	54(5)	18(3)	0(3)	11(3)
O(13)	47(4)	34(4)	61(6)	-13(3)	12(4)	-11(3)
O(14)	68(5)	32(4)	52(5)	-10(3)	-20(4)	2(3)
O(15)	115(8)	109(7)	50(6)	-43(5)	27(5)	-61(6)
O(16)	32(3)	63(4)	24(4)	-12(3)	2(3)	-21(3)
O(17)	59(5)	50(4)	36(5)	-10(3)	-2(4)	11(3)
O(18)	11(4)	318(15)	62(7)	-110(9)	-15(4)	24(6)
O(19)	81(6)	177(10)	132(10)	-136(9)	18(6)	-37(7)
N(1)	27(4)	7(3)	37(5)	-1(3)	7(3)	-4(3)
N(2)	37(4)	18(4)	25(5)	-8(3)	-8(4)	3(3)
N(3)	20(4)	27(4)	20(5)	4(3)	-4(3)	-1(3)
N(4)	17(4)	21(4)	29(5)	0(3)	2(3)	2(3)

N(5)	51(5)	13(4)	94(8)	-19(4)	-54(5)	15(3)
N(6)	42(5)	19(4)	86(8)	3(4)	-44(5)	-4(4)
N(7)	20(4)	58(5)	16(5)	0(4)	0(3)	-1(3)
N(8)	23(4)	19(3)	25(5)	-2(3)	-1(3)	4(3)
C(1)	20(5)	22(5)	65(8)	11(5)	-4(5)	8(4)
C(2)	32(5)	41(5)	24(6)	8(4)	-21(4)	-3(4)
C(3)	30(5)	35(5)	35(7)	-6(4)	-16(5)	-3(4)
C(5)	32(5)	23(5)	39(7)	-6(4)	2(4)	4(4)
C(6A)	40(5)	13(4)	25(6)	-11(4)	-5(4)	-2(4)
C(6)	20(5)	30(5)	43(7)	10(4)	-3(4)	10(4)
C(7)	17(4)	31(5)	54(8)	-5(5)	0(5)	6(4)
C(8)	18(4)	43(5)	24(6)	6(4)	9(4)	-4(4)
C(9)	16(4)	30(5)	42(7)	-3(4)	8(4)	-3(4)
C(10)	36(5)	18(4)	42(7)	1(4)	3(5)	-4(4)
C(11)	34(5)	37(5)	19(6)	2(4)	3(4)	12(4)
C(12)	41(5)	39(5)	15(6)	-9(4)	-6(4)	6(4)
C(13)	28(5)	16(4)	52(7)	-10(4)	11(5)	-2(4)
C(14)	20(4)	35(5)	23(6)	14(4)	-8(4)	-10(4)
C(15)	117(11)	4(5)	227(19)	-9(7)	-134(13)	0(6)
C(16)	101(10)	19(5)	177(16)	-16(7)	-116(11)	8(6)
C(17)	51(8)	81(9)	78(11)	55(8)	-42(7)	-40(7)
C(18)	24(5)	104(10)	25(7)	21(6)	-2(5)	-27(6)
C(19)	23(5)	47(6)	46(7)	-29(5)	-2(5)	12(4)
C(20)	34(5)	37(5)	47(7)	-23(5)	-15(5)	7(4)
C(21)	17(4)	29(5)	36(6)	-7(4)	-9(4)	-3(4)
C(22)	18(4)	33(5)	30(6)	-7(4)	-7(4)	-1(4)
C(23)	36(5)	25(5)	66(8)	3(5)	-31(5)	-3(4)
C(24)	54(7)	23(5)	101(12)	-4(6)	-54(7)	4(5)
C(25)	35(6)	65(7)	50(9)	27(6)	-15(6)	-29(5)
C(26)	12(4)	83(8)	34(7)	-2(6)	-4(4)	0(5)
C(27)	53(7)	88(9)	101(12)	-75(8)	-56(7)	52(6)
C(28)	17(4)	36(5)	39(7)	10(4)	-6(4)	-9(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^{-3}) for wong188.

	x	y	z	U(eq)
H(1A)	300	6002	7766	46
H(1B)	604	6928	7182	46
H(2A)	2074	6218	6232	39
H(2B)	432	5940	6363	39
H(3A)	963	4659	7284	39
H(3B)	1589	4673	6350	39
H(5A)	5345	3679	7344	38
H(5B)	4378	3058	8081	38
H(6A)	3277	3532	6889	30
H(6B)	2355	3646	7737	30
H(6C)	6714	3998	8425	40
H(6D)	6267	4913	8685	40
H(7A)	7987	4961	7433	42
H(7B)	6674	4734	7018	42
H(8A)	6765	6266	7729	37
H(8B)	7331	6272	6788	37
H(9A)	5327	7484	6704	37
H(9B)	5070	7196	7672	37
H(10A)	2978	7775	7348	40
H(10B)	2996	7233	6624	40
H(11A)	5863	6015	5912	37
H(11B)	4322	6424	6038	37
H(12A)	3866	5066	5826	37
H(12B)	5019	4635	6354	37
H(13A)	955	6372	8809	41
H(13B)	1509	7359	8463	41
H(14A)	4402	4336	9515	33
H(14B)	4505	3365	9320	33
H(15A)	217	2276	7408	127
H(15B)	-605	2630	8185	127
H(16A)	-2802	2147	7946	107
H(16B)	-2024	2683	7094	107
H(17A)	-161	1817	6470	90
H(17B)	-1329	1644	5931	90

H(18A)	-885	208	6047	66
H(18B)	657	658	5922	66
H(19A)	15	-1271	7584	44
H(19B)	204	-1131	6613	44
H(20A)	-2166	-897	6600	44
H(20B)	-2121	-1720	7306	44
H(21A)	-4833	-167	7820	32
H(21B)	-4528	-822	7185	32
H(22A)	-3108	312	6266	32
H(22B)	-4751	536	6434	32
H(23A)	-4184	1372	7414	50
H(23B)	-3607	1777	6488	50
H(24A)	1660	1563	8424	67
H(24B)	1276	543	8657	67
H(25A)	2883	1009	7425	64
H(25B)	1558	1432	7042	64
H(26A)	2175	6	6745	53
H(26B)	1646	-381	7681	53
H(28A)	-3616	-1779	8416	39
H(28B)	-4108	-945	8821	39

X-ray Crystallographic Software Employed:

APEX2 Version 2.2 /SHELXTL (Bruker AXS Inc., 2007)
SAINT Version 7.34a (Bruker AXS Inc., 2007)
SADABS Version 2007/2 (Sheldrick, Bruker AXS Inc.)
XPREP Version 2005/2 (Sheldrick, Bruker AXS Inc.)

Bruker suite of programs APEX2/SHELXTL, SAINT, SADABS, XPREP may be obtained from Bruker AXS.Inx, 5467 East Cheryl Parkway, Madison WI 53711

XS Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) **A64**, 112-122.)
XL Version 2008/1 (George M. Sheldrick, Acta Cryst. (2008) **A64**, 112-122.)

X-ray crystal structure figures were prepared using CrystalMaker 8.2 for Mac (CrystalMaker Software Ltd., Centre for Innovation & Enterprise, Oxford University Begbroke Science Park, Sandy Lane, Yarnton, Oxfordshire, OX5 1PF, UK; http://www.crystalmaker.com)

Biodistribution of ^{64}Cu-**2**:

Biodistribution of ^{64}Cu-CB-TE2P in 33 male Lewis rats; 1, 2, 4, & 24 hr (%ID/gram)

	1 Hr.			2 Hr.			4 Hr.			24 Hr.		
blood	0.1515	+/-	0.0247	0.0208	+/-	0.0046	0.0030	+/-	0.0005	0.0019	+/-	0.0004
lung	0.1274	+/-	0.0336	0.0379	+/-	0.0045	0.0408	+/-	0.0269	0.0126	+/-	0.0024
liver	0.0929	+/-	0.0062	0.0741	+/-	0.0093	0.0594	+/-	0.0057	0.0274	+/-	0.0015
spleen	0.0474	+/-	0.0096	0.0243	+/-	0.0024	0.0222	+/-	0.0038	0.0172	+/-	0.0010
kidney	1.1894	+/-	0.3496	0.4912	+/-	0.0713	0.4285	+/-	0.0306	0.3568	+/-	0.0517
muscle	0.0600	+/-	0.0092	0.0151	+/-	0.0029	0.0085	+/-	0.0021	0.0068	+/-	0.0012
fat	0.0578	+/-	0.0118	0.0158	+/-	0.0033	0.0060	+/-	0.0041	0.0003	+/-	0.0032
heart	0.0731	+/-	0.0204	0.0172	+/-	0.0071	0.0144	+/-	0.0062	0.0080	+/-	0.0006
bone	0.6862	+/-	0.1429	0.3087	+/-	0.0296	0.1676	+/-	0.0131	0.1186	+/-	0.0159
marrow	0.1199	+/-	0.0205	0.0643	+/-	0.0099	0.0290	+/-	0.0107	0.0120	+/-	0.0149
stomach	0.0825	+/-	0.0316	0.0389	+/-	0.0135	0.0464	+/-	0.0202	0.0262	+/-	0.0312
sm int	0.1064	+/-	0.0619	0.0472	+/-	0.0189	0.0289	+/-	0.0066	0.0135	+/-	0.0043
u lg int	0.2452	+/-	0.0540	0.1562	+/-	0.0513	0.2507	+/-	0.0873	0.0354	+/-	0.0175
l lg int	0.0285	+/-	0.0029	0.0562	+/-	0.0400	0.1448	+/-	0.0480	0.1736	+/-	0.0453
tail	0.4413	+/-	0.3154	0.1852	+/-	0.1090	0.2824	+/-	0.3877	0.0932	+/-	0.0386