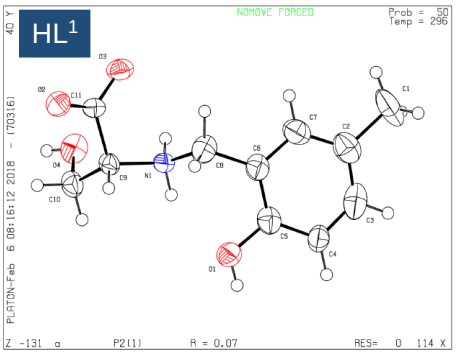
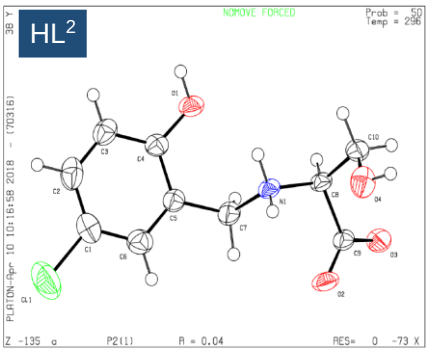
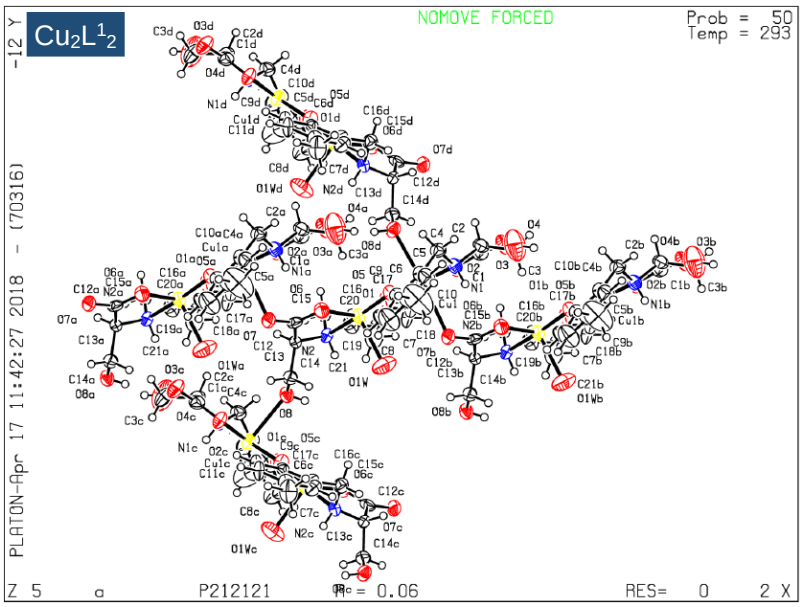
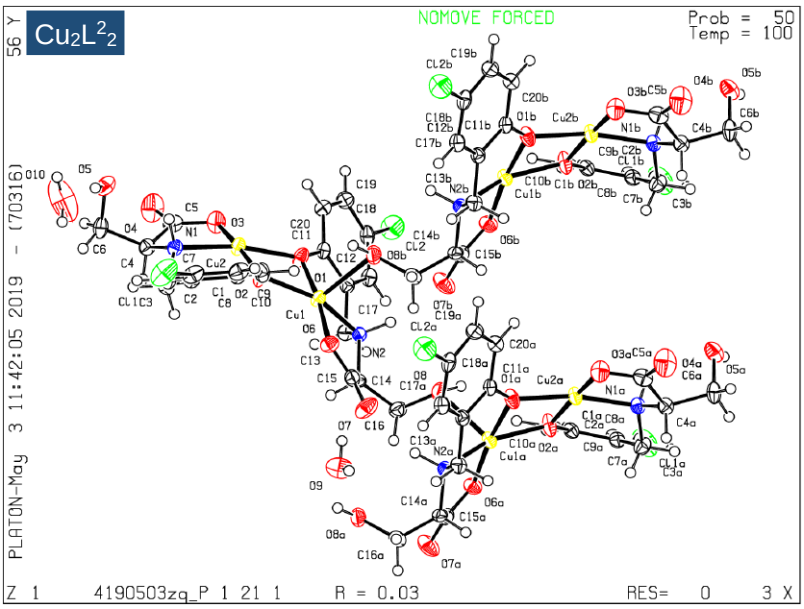
Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information









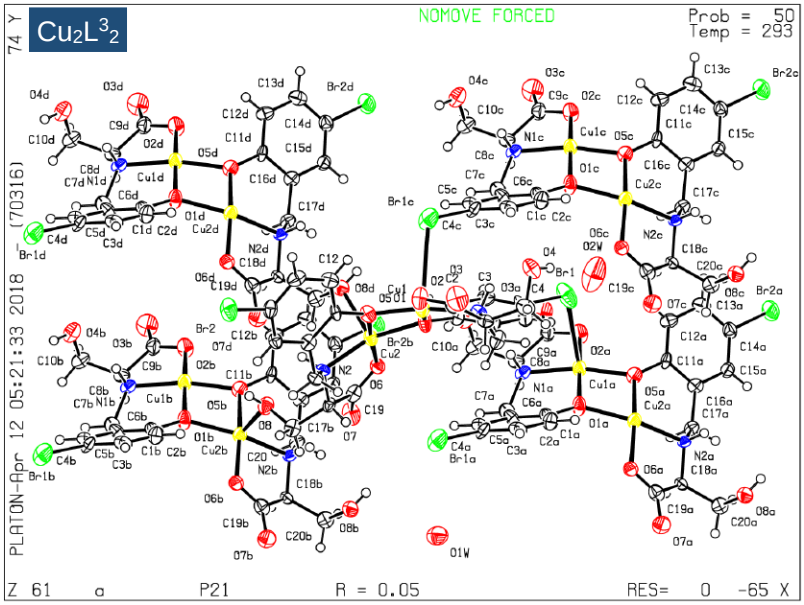


Figure S-1. Collected crystal structures of the two reduced L-serine Schiff bases and three binuclear copper(II) complexes with reduced L-serine Schiff bases.

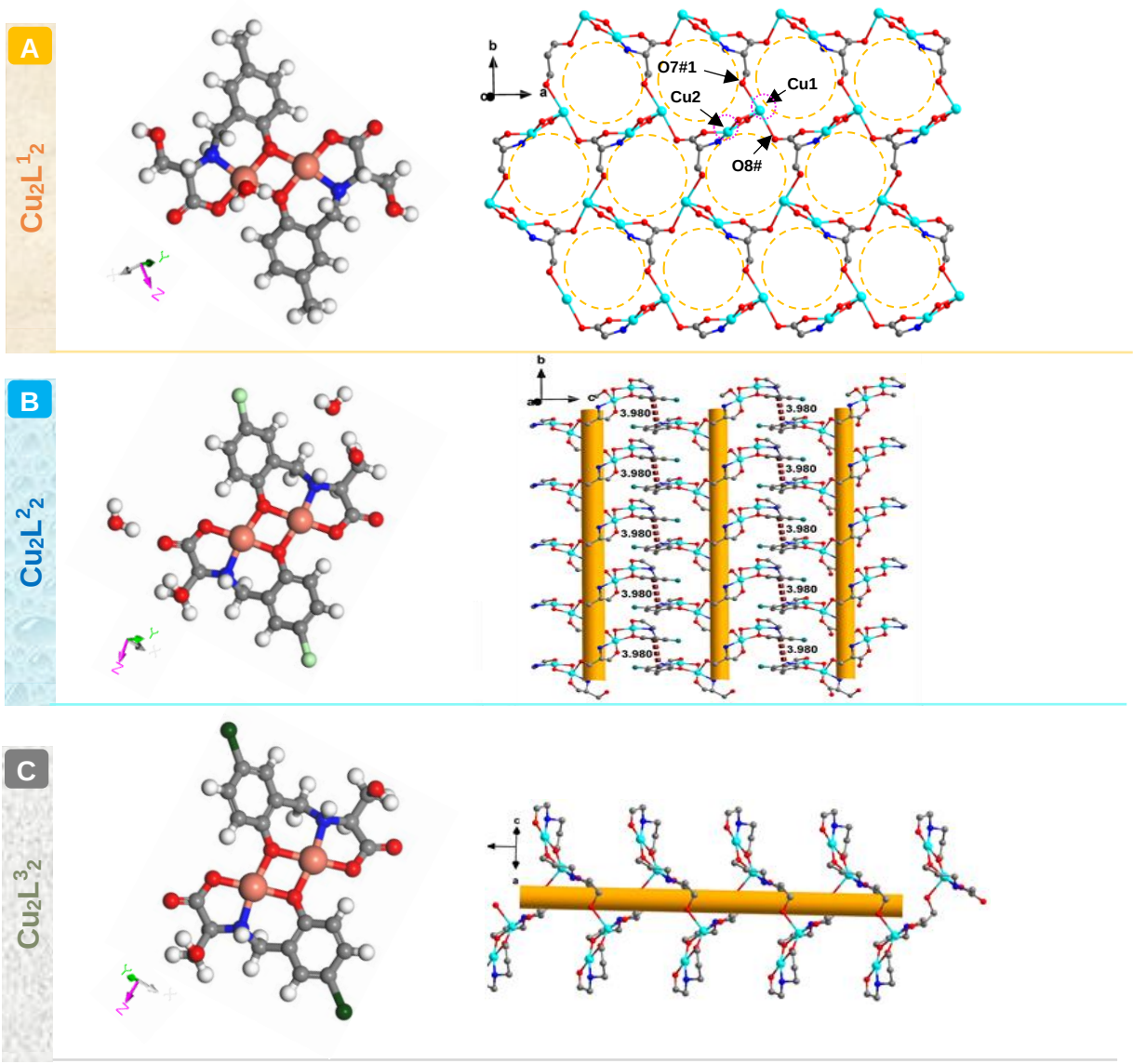


Figure S-2. Molecule structures (left column) and topological structures (right column) of binuclear copper(II) complexes with reduced L-serine Schiff bases.

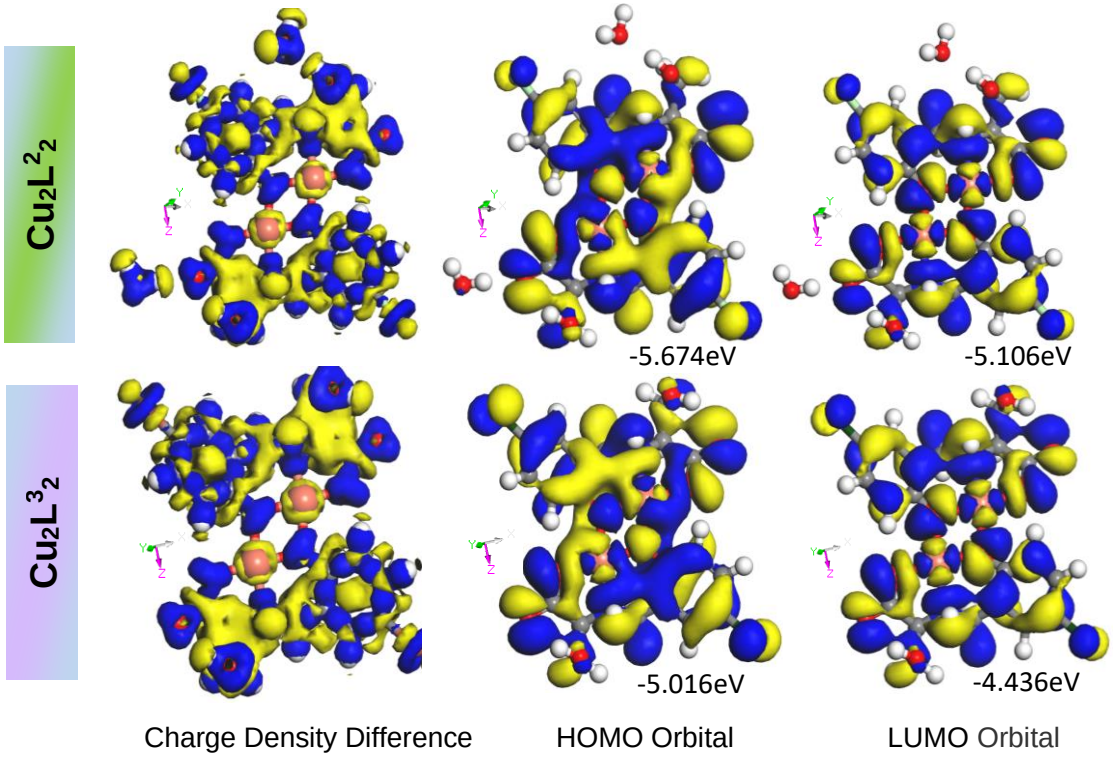


Figure S-3. Representations of the charge density difference (left column), HOMO (central column) and LUMO (right column) orbitals for $Cu_2L^2_2$ and $Cu_2L^3_2$.

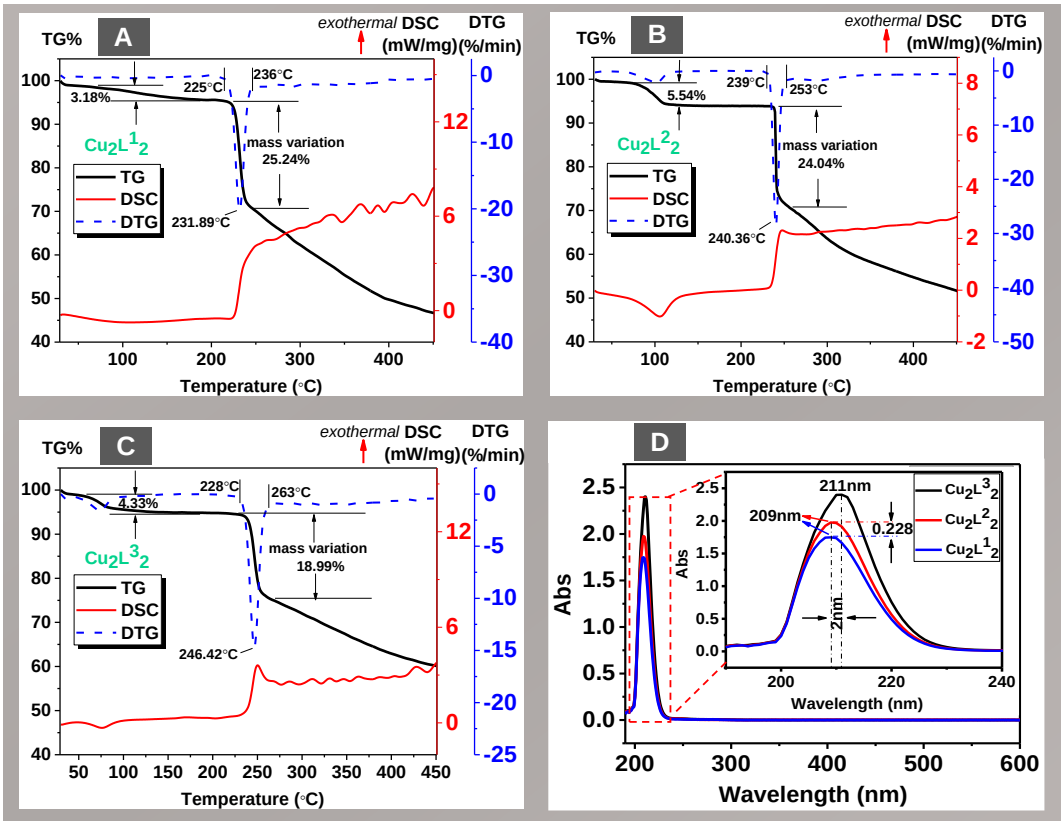


Figure S-4. Thermal analysis (A-C) and electronic spectra (D) of three binuclear copper(II) complexes used in this work. Thermal analysis was performed in the range of 30 °C to 451°C. Electronic spectra were recorded in buffered aqueous solution under a selected condition (25°C, pH 7.0, $C_{complex}=6.67\times10^{-6}$ mol L^{-1}).

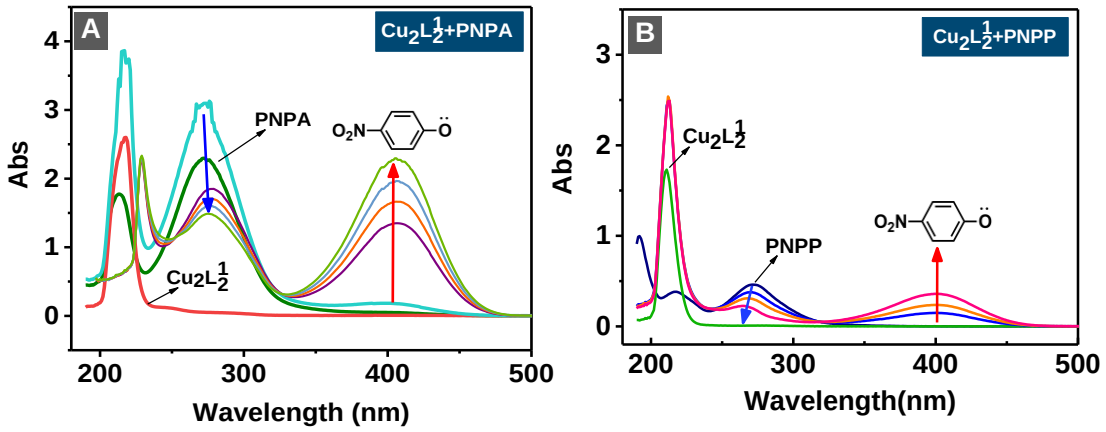
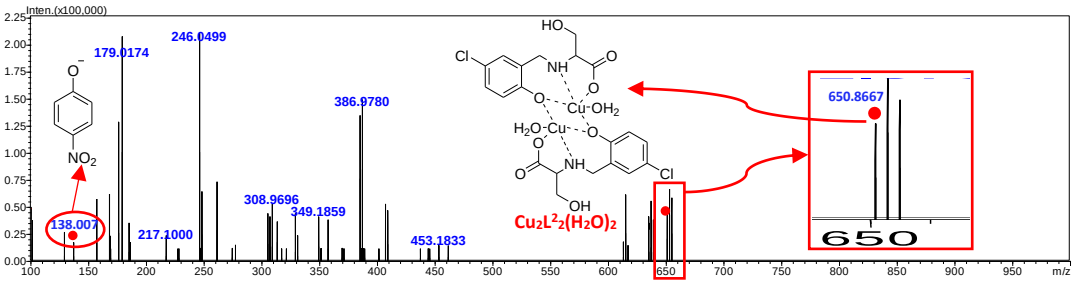


Figure S-5. Representative UV-vis absorbance scan for the hydrolysis of PNPA (A) and PNPP (B) by $Cu_2L^1_2$.

(1) PNPA+$Cu_2L^2_2$



(2) PNPP+$Cu_2L^2_2$

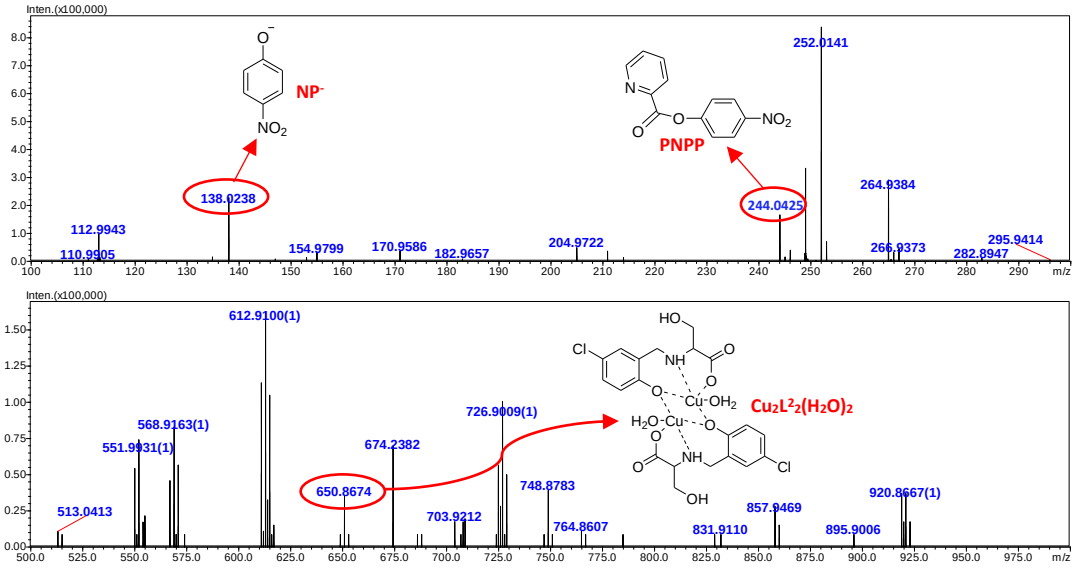


Figure S-6. ESI-MS spectra for the hydrolysis of PNPP or PNPA promoted by $Cu_2L^2_2$.

Table S-1 Crystal parameters of binuclear copper(II) complexes with reduced Schiff bases

Complex	$Cu_2L^1_2$	$Cu_2L^2_2$	$Cu_2L^3_2$
Empirical formula	$C_{22}H_{26}Cu_2N_2O_9$	$C_{20}H_{24}Cl_2Cu_2N_2O_{10}$	$C_{20}H_{20}Br_2Cu_2N_2O_{10}$
Formula wt.	589.53	650.41	735.28
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	P $2_12_12_1$/c	P 2_1/c	P 2_1/c
a (Å)	7.527(4)	11.570(4)	11.541(6)
b (Å)	14.125(8)	7.832(3)	7.848(4)
c (Å)	23.965(13)	13.325(5)	13.547(7)
α (deg)	90.00	90.000	90.000
β (deg)	90.00	99.669	98.201(9)
γ (deg)	90.00	90.000	90.000
h, k, l $_{max}$	8, 16, 28	14, 10, 17	13, 9, 16
V (Å^3)	2548(2)	1190.3(8)	1214.5(11)
μ (mm^{-1})	1.721	2.071	5.099
Z	4	2	2
D_c (g/cm^3)	1.537	1.540	2.011
F (000)	1208	660	724
Reflections collected	4468	4037	4038
Reflections with I >2σ (I)	3032	3260	3174
R (int)	0.0886	0.0322	0.0400
R1[I>2σ (I)]*	0.0596	0.0333	0.0451
wR2[I>2σ (I)]**	0.1180	0.0702	0.0914
R1 (all data)*	0.0985	0.0387	0.0641
wR2 (all data)**	0.1292	0.0724	0.0985

Equation * $R = \sum (F_o - F_c)/\sum(F_o)$ ** $wR = \{\sum[w(F_o^2 - F_c^2)^2]/\sum(F_o^2)^2\}^{1/2}$

Table S-2 Selected bond lengthen(Å) and angle (deg) of binuclear copper(II) complexes

$Cu_2L^1_2$			
Cu(1)-O(1)	1.928(5)	Cu(1)-O(2)	1.932(6)
Cu(1)-O(5)	1.978(6)	Cu(1)-N(1)	1.969(6)
Cu(2)-O(1)	1.918(5)	Cu(2)-O(5)	1.965(5)
Cu(2)-O(6)	1.944(6)	Cu(2)-O(8)	2.307(6)
Cu(2)-N(2)	1.966(6)	Cu(2)-Cu(1)	2.993(19)
O(1)-Cu(1)-O(2)	176.2(2)	O(1)-Cu(1)-O(5)	78.9(2)
O(2)-Cu(1)-O(5)	103.3(2)	O(1)-Cu(1)-N(1)	93.2(2)
O(2)-Cu(1)-N(1)	84.7(3)	O(5)-Cu(1)-N(1)	172.0(3)
O(1)-Cu(2)-O(1)	91.5(2)	O(1)-Cu(2)-O(5)	80.1(2)
O(1)-Cu(2)-O(6)	98.1 (2)	O(5)-Cu(2)-O(6)	150.1(2)
O(5)-Cu(2)-O(6)	150.1(2)	O(5)-Cu(2)-O(1)	99.6(3)
O(1)-Cu(2)-N(2)	93.3(3)	O(1)-Cu(2)-N(2)	173.1(2)
O(5)-Cu(2)-N(1)	94.1(3)	O(6)-Cu(2)-N(2)	85.0(3)
$Cu_2L^2_2$			
Cu(1)-O(1)	1.943(3)	Cu(2)-O(2)	1.930(3)
Cu(1)-O(2)	1.955(3)	Cu(2)-O(1)	1.940(3)
Cu(1)-O6	1.927(3)	Cu(2)-O(3)	1.906(3)
Cu(1)-O(8)	2.345(3)	Cu(2)-N(1)	1.968(4)
Cu(1)-N(2)	1.998(4)	Cu(1)-Cu(2)	3.001 (10)
O(2)-Cu(1)-O(8)	106.12(14)	O6-Cu(1)-O(2)	100.07(14)
O(2)-Cu(1)-N(2)	155.99(16)	O6-Cu(1)-O(1)	172.48(16)
O(1)-Cu(1)-O(2)	77.10(13)	O6-Cu(1)-O(8)	88.03(14)
O(1)-Cu(1)-O(8)	99.44(15)	O6-Cu(1)-N(2)	85.64(15)
O(1)-Cu(1)-N(2)	94.22(14)	N(2)-Cu(1)-O(8)	97.32(14)
O(2)-Cu(2)-O(1)	77.76(13)	O(3)-Cu(2)-O(2)	175.41(17)
O(2)-Cu(2)-N(1)	94.39(14)	O(3)-Cu(2)-O(1)	100.82(14)
O(1)-Cu(2)-N(1)	168.61(17)	O(3)-Cu(2)-N(1)	86.36(15)
$Cu_2L^3_2$			
Cu(1)-O(1)	1.928(5)	Cu(1)-O(2)	1.911(6)
Cu(1)-O(5)	1.925(5)	Cu(1)-N(1)	1.972(6)
Cu(2)-O(1)	1.965(5)	Cu(2)-O(5)	1.943(5)
Cu(2)-O(6)	1.945(6)	Cu(2)-O(8)	2.335(6)
Cu(2)-N(2)	1.995(6)	Cu(2)-Cu(1)	3.008(16)
O(1)-Cu(1)-O(2)	176.5(3)	O(1)-Cu(1)-O(5)	78.0(2)
O(2)-Cu(1)-O(5)	101.9(2)	O(1)-Cu(1)-N(1)	93.5(2)
O(2)-Cu(1)-N(1)	86.1(2)	O(5)-Cu(1)-N(1)	168.49(3)
O(1)-Cu(2)-O(5)	76.7(2)	O(1)-Cu(2)-O(6)	100.1(2)
O(1)-Cu(2)-O(8)	107.2(2)	O(5)-Cu(2)-O(6)	172.6(3)
O(5)-Cu(2)-O(8)	99.0(2)	O(6)-Cu(2)-O(8)	88.3(2)
O(1)-Cu(2)-N(2)	155.3(3)	O(5)-Cu(2)-N(2)	94.5(2)
O(6)-Cu(2)-N(2)	85.8(2)	O(8)-Cu(2)-N(2)	96.9(2)

Table S-3 Calculated Addison Tau factors (τ) and geometry for the central copper(II) of binuclear copper(II) complexes

Catalyst	Cu(1)		Cu(2)	
	τ	Geometrical shape	τ	Geometrical shape
$Cu_2L^1_2$	0.08	octahedral	0.26	distorted tetrahedral
$Cu_2L^2_2$	0.22	distorted tetrahedral	0.11	distorted square planar
$Cu_2L^3_2$	0.11	distorted square planar	0.23	distorted tetrahedral

Table S-4 Calculated Mulliken charges of the two copper (II) centers of binuclear copper(II) complexes

$Cu_2L^1_2$		**$Cu_2L^2_2$**		**$Cu_2L^3_2$**	
Cu(1)	Cu(2)	Cu(1)	Cu(2)	Cu(1)	Cu(2)
0.573	0.569	0.576	0.586	0.58	0.581

Table S-5 Relative activities of PNPP hydrolysis between various catalytic systems

Catalyst	**Relative Activity**	
None	CTAB/Buffer	
	11.48	
$Cu_2L^1_2$	($Cu_2L^1_2$+CTAB)/CTAB	$Cu_2L^1_2$/CTAB
	1206	605.2
$Cu_2L^2_2$	($Cu_2L^2_2$+CTAB)/CTAB	$Cu_2L^2_2$/CTAB
	1050	336.4
$Cu_2L^3_2$	($Cu_2L^3_2$+CTAB)/CTAB	$Cu_2L^3_2$/CTAB
	1039	337.9