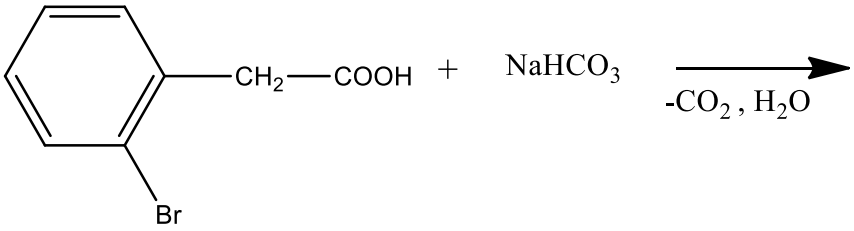
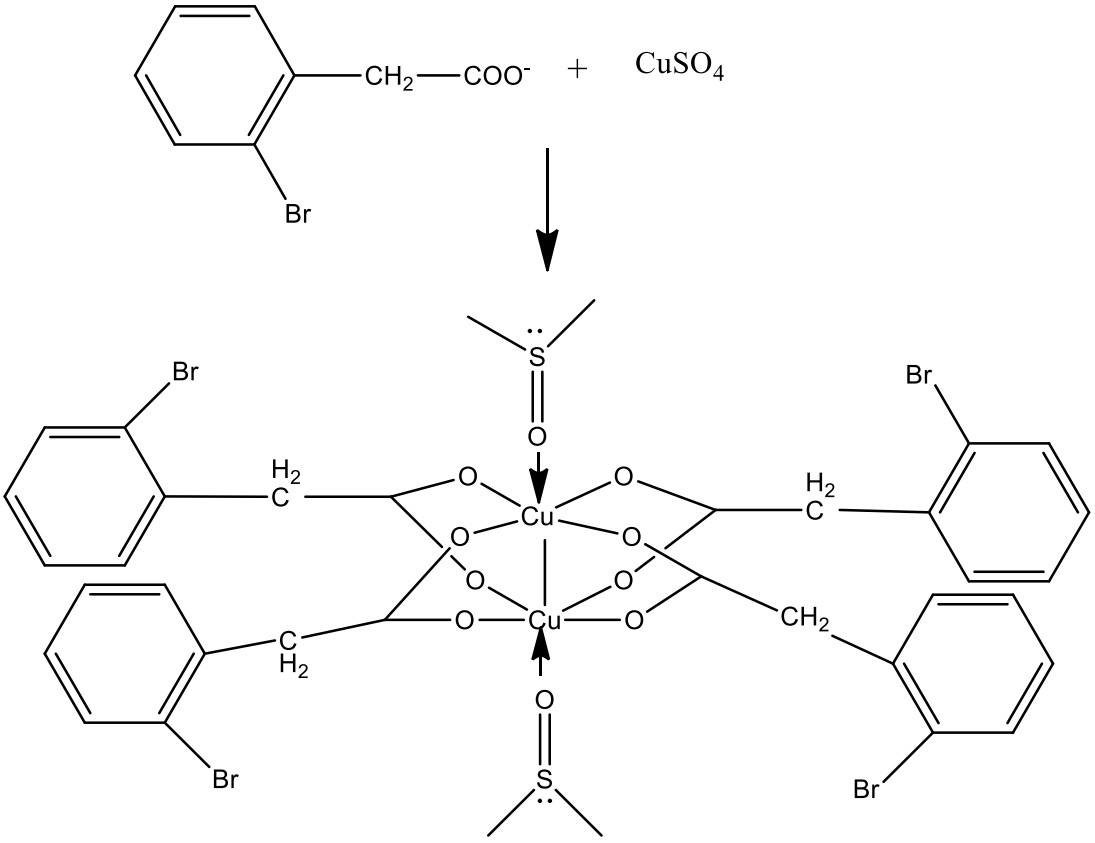
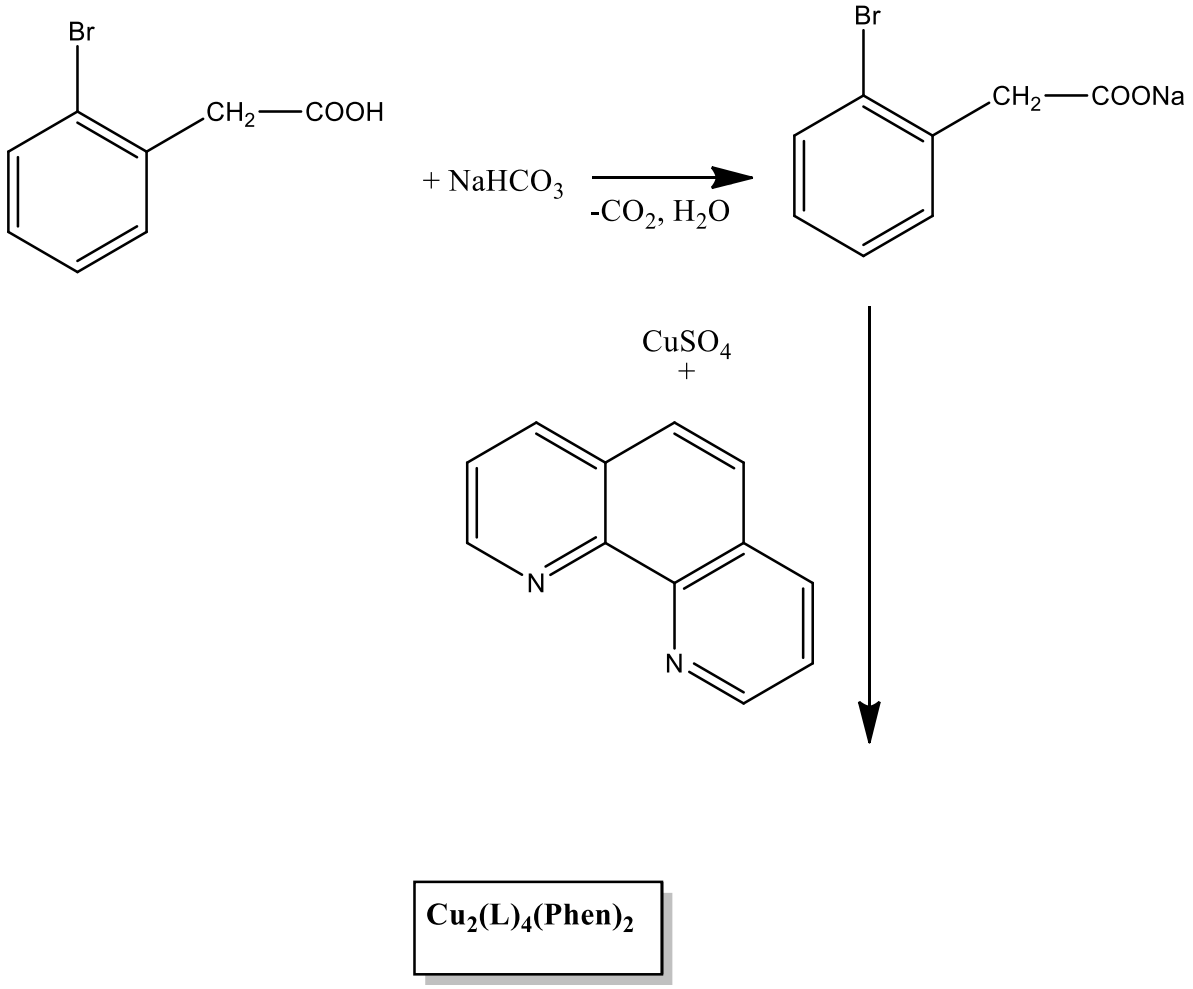
Binuclear copper(II) complexes: synthesis, structural characterization, DNA binding and *in silico* studies

Supplementary material





Scheme S1. Synthesis of complex 1



Where L= 2-bromophenyl acetate and Phen= 1,10- phenanthroline

Scheme S2. Synthesis of complex 2

Table S1. Crystal data and structure refinement parameters for complexes

Parameter	**1**	**2**
Empirical formula	$C_{56}H_{40}Br_4Cu_2N_4O_8$	$C_{56}H_{40}Br_4Cu_2N_4O_8$
Formula weight, g mol^{-1}	1139.48	1343.64
Temperature, K	296(2)	296(2)
Wavelength, Å	0.71073	0.71073
Crystal system	Triclinic	Monoclinic
Space group	P -1	C 2/c
Unit cell dimensions		

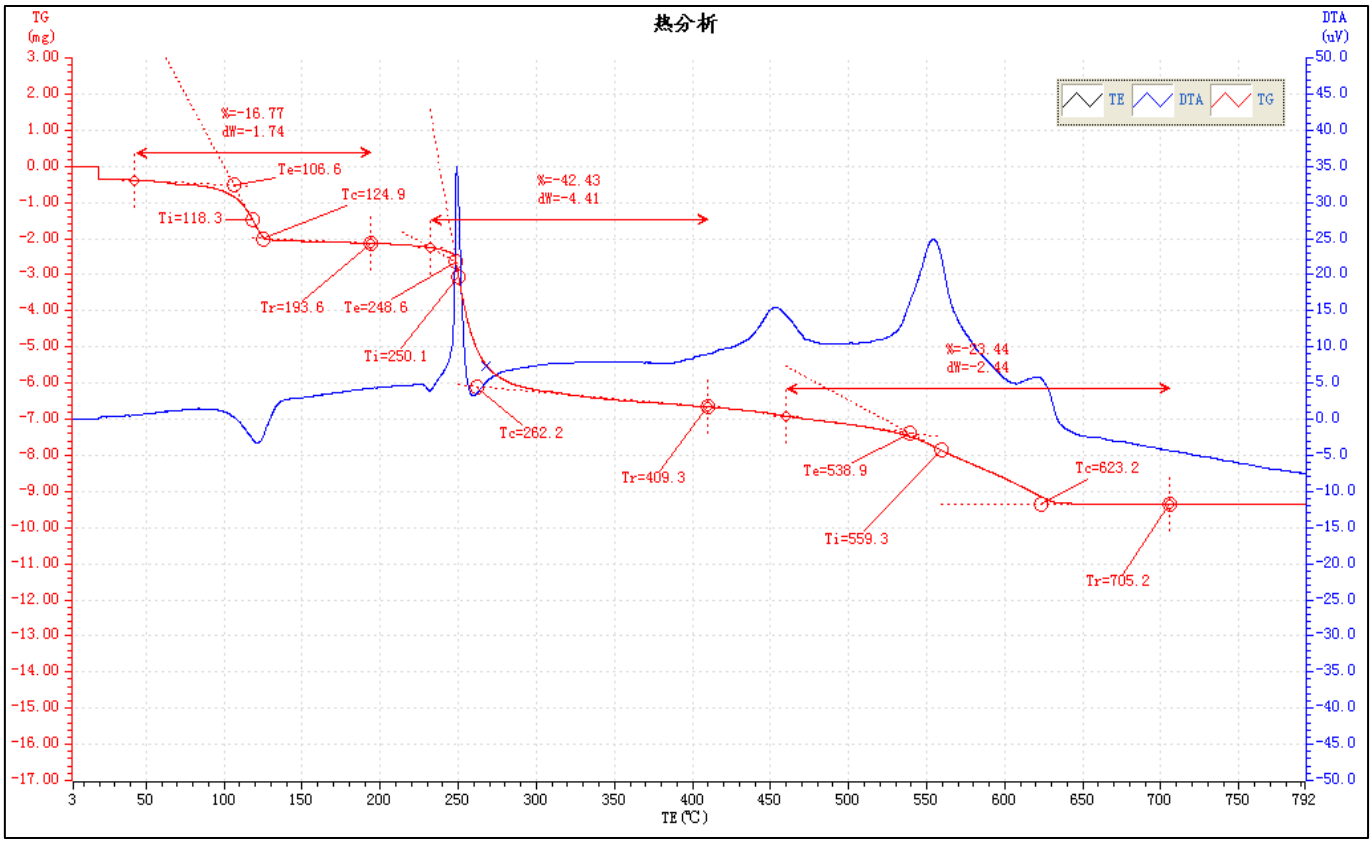
a / Å	8.3934(8)	29.194(3)
b / Å	10.5368(9)	10.9925(6)
c / Å	12.8600(13)	20.352(2)
α / °	89.424(3)	90
β / °	73.408(2)	130.365(2)
γ / °	72.498(3)	90
Volume, $Å^3$	1035.94(17)	4976.4(8)
Z	2	4
Density (calculated), Mg/m^3	1.827	1.793
Absorption coefficient, mm^{-1}	5.038	4.129
F(000)	562	2664
Crystal size (mm^3)	0.44 × 0.32 × 0.28	0.38 × 0.18 × 0.16
θ range for data collection (°)	2.515 to 27.946	2.627 to 27.960
Index ranges	-11 ≤ h ≤ 11	-38 ≤ h ≤ 36
	-12 ≤ k ≤ 13	-14 ≤ k ≤ 11
	-14 ≤ l ≤ 16	-21 ≤ l ≤ 26
Reflections collected	11991	16671
Independent reflections	4912 [R(int) = 0.0465]	5914 [R(int) = 0.0425]
Completeness to θ (%)	99.4	99.6
Refinement method	Full-matrix LS on F^2	Full-matrix LS on F^2
Data / restraints / parameters	4912/ 0 / 246	5914/ 0 / 334
Goodness-of-fit on F^2	1.040	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0440, wR2 = 0.1087	R1 = 0.0355, wR2 = 0.0801
R indices (all data)	R1 =0.0664, wR2 = 0.1207	R1 =0.0612, wR2 = 0.0886

Table S2: selected bond lengths and angles of complexes

Complex	**1**	**2**
	Distances, Å	
Cu(1)-O(1)	1.976(2)	1.9298(17)
Cu(1)-O(2)	1.967(2)	---

Cu(1)-O(3)	1.961(2)	1.9547(17)
Cu(1)-O(4)	1.959(2)	---
Cu(1)-O(5)	2.153(2)	---
Cu(1)-N(1)	---	2.037(2)
Cu(1)-N(2)	---	2.037(2)
	Angles, °	
O(1)-Cu(1)-O(2)	167.80(9)	---
O(1)-Cu(1)-O(3)	90.15(11)	95.96(8)
O(1)-Cu(1)-N(2)	---	89.71(8)
O(3)-Cu(1)-N(2)	---	168.35(8)
O(1)-Cu(1)-N(1)	---	169.12(8)
O(3)-Cu(1)-N(1)	---	94.50(8)
N(2)-Cu(1)-N(1)	---	80.53(8)
O(1)-Cu(1)-O(4)	88.69(11)	---
O(3)-Cu(1)-O(4)	167.91(9)	---
O(2)-Cu(1)-O(4)	89.50(11)	---
O(2)-Cu(1)-O(3)	89.10(11)	---
O(5)-Cu(1)-O(3)	94.04(10)	---
O(5)-Cu(1)-O(4)	98.03(10)	---
O(5)-Cu(1)-O(1)	98.93(10)	---
O(5)-Cu(1)-O(2)	93.27(10)	---

Figure S1: TG curve of complex 1



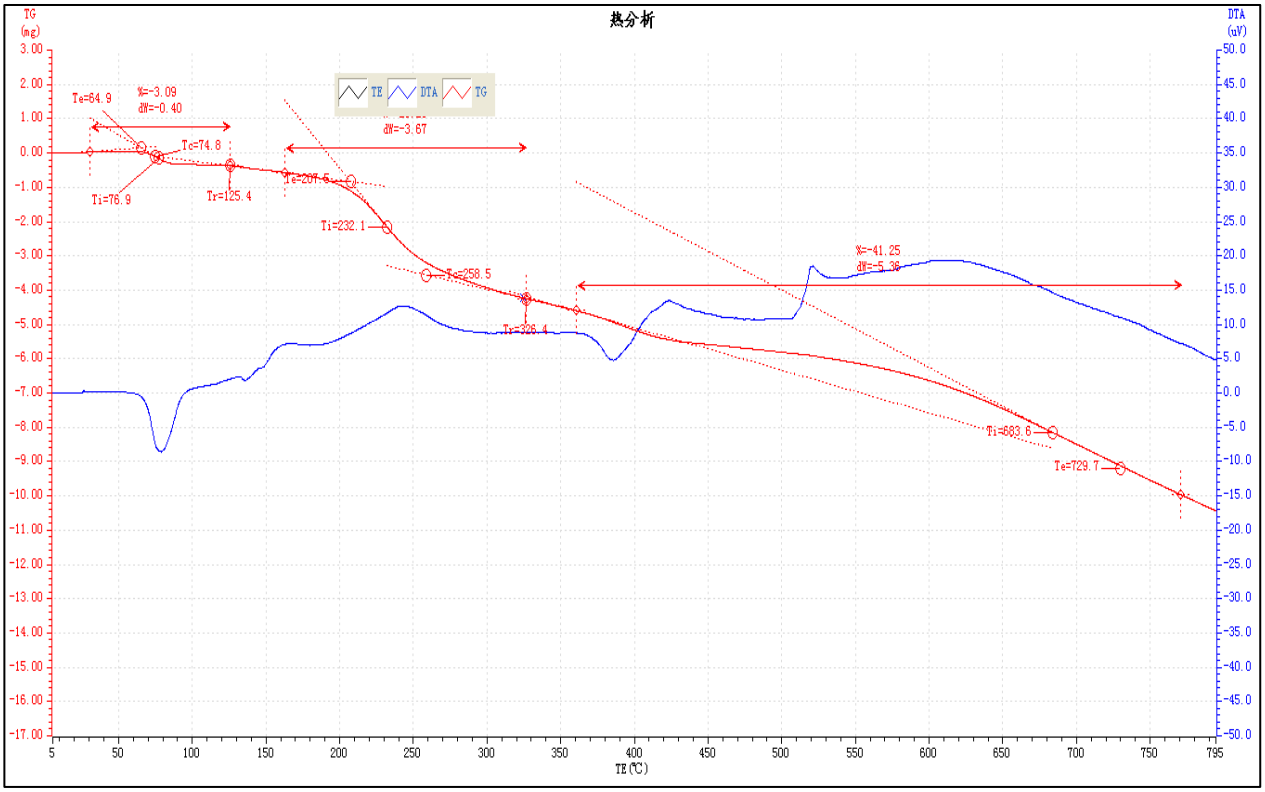


Figure S2: TG curve of complex 2