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Supplementary material

SUPPLEMENTARY MATERIAL TO

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

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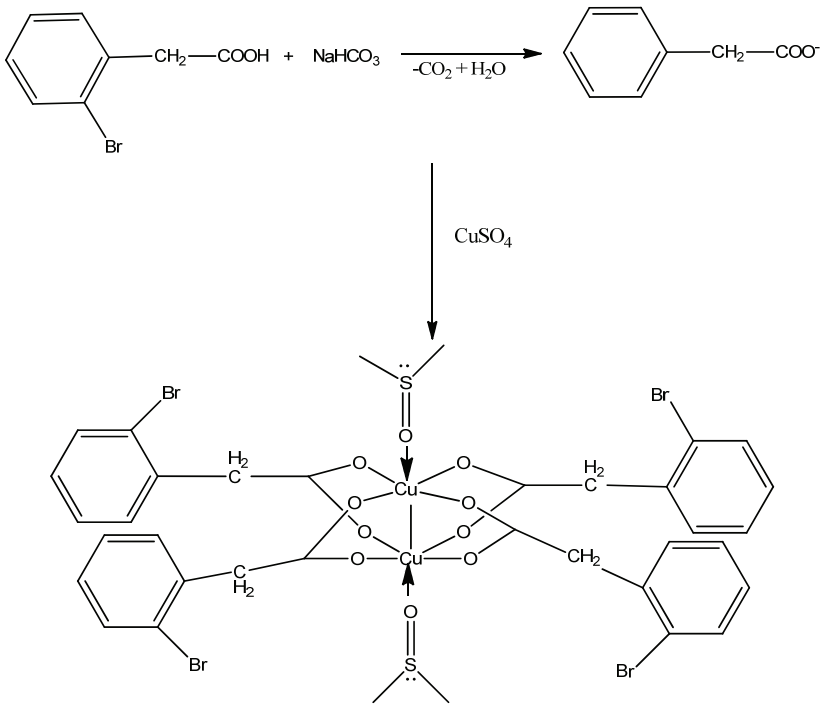

Scheme S-1. Synthesis of complex **1**.

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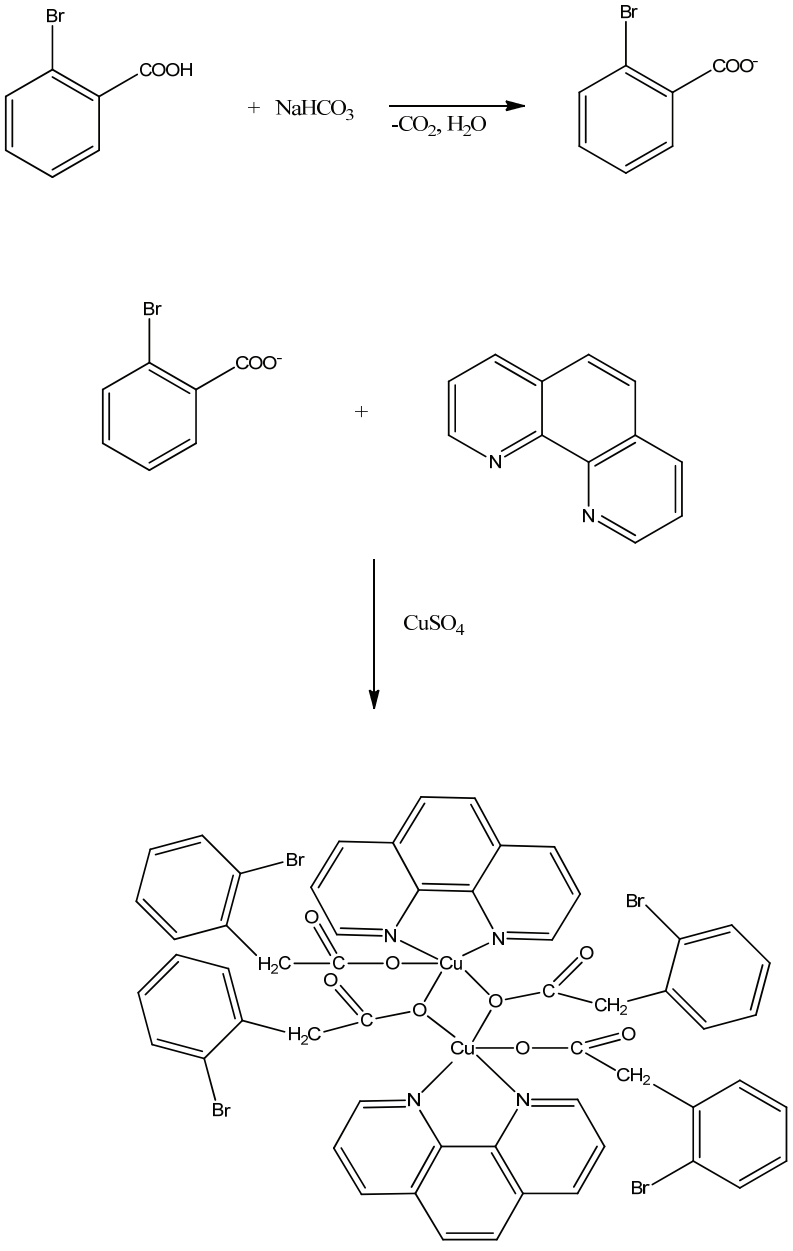

Scheme S-2. Synthesis of complex **2**.

TABLE S-I. 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	$-11 \le h \le 11$ $-12 \le k \le 13$ $-14 \le l \le 16$	$-38 \le h \le 36$ $-14 \le k \le 11$ $-21 \le l \le 26$
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 S-II. 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)	---

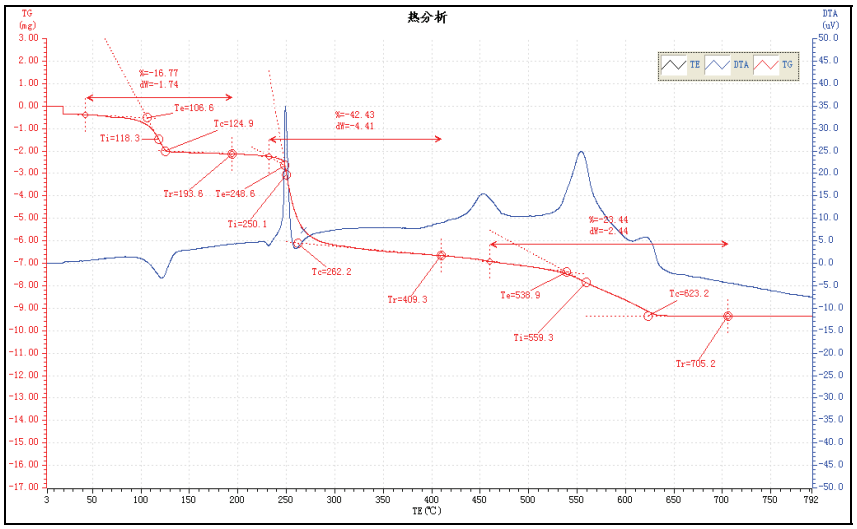

Fig. S-1. TG curve of complex **1**.

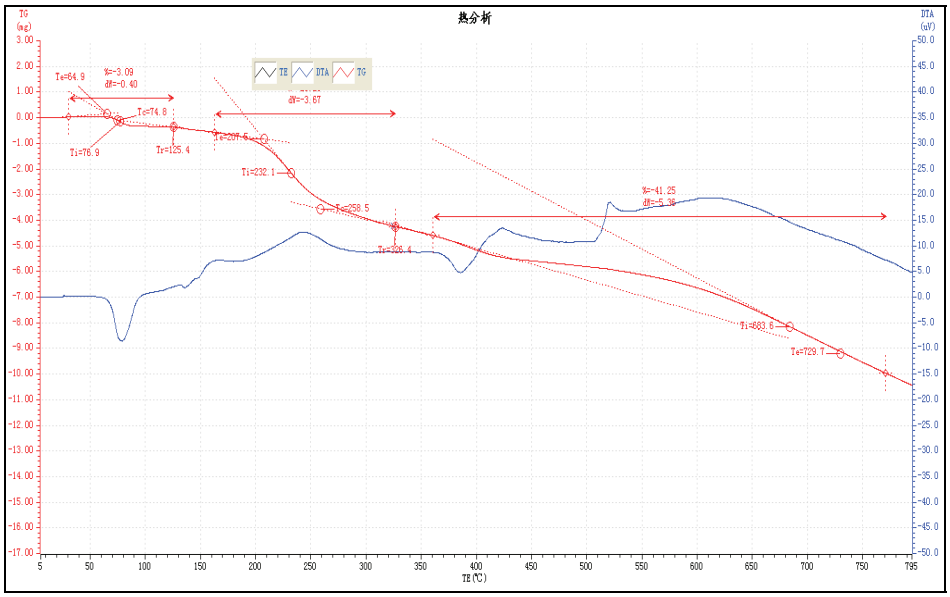

Fig. S-2. TG curve of complex **2**.