

## SUPPLEMENTARY MATERIAL

### Synthesis, structure and magnetic characterization of dinuclear copper(II) complexes bridged by bicompartamental phenolate

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ESI  
-19255 ✓

#2700

✓

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Comment  
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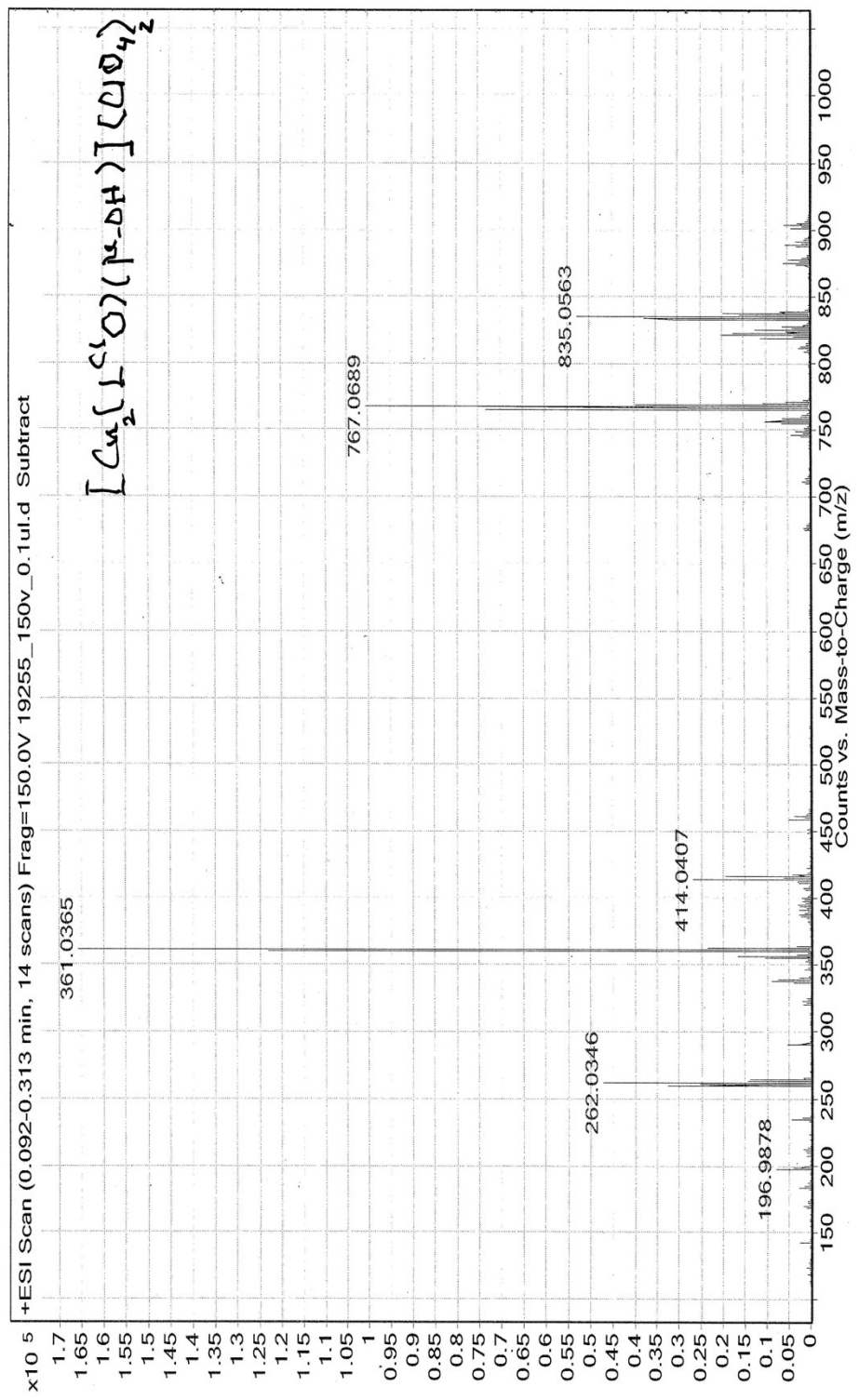


Fig. S1. ESI Mass spectrum of  $[Cu_2(\mu-L^{ClO})(\mu-OH)](ClO_4)_2$  (1) in acetonitrile solution

EST  
# 21375

POS

#2666

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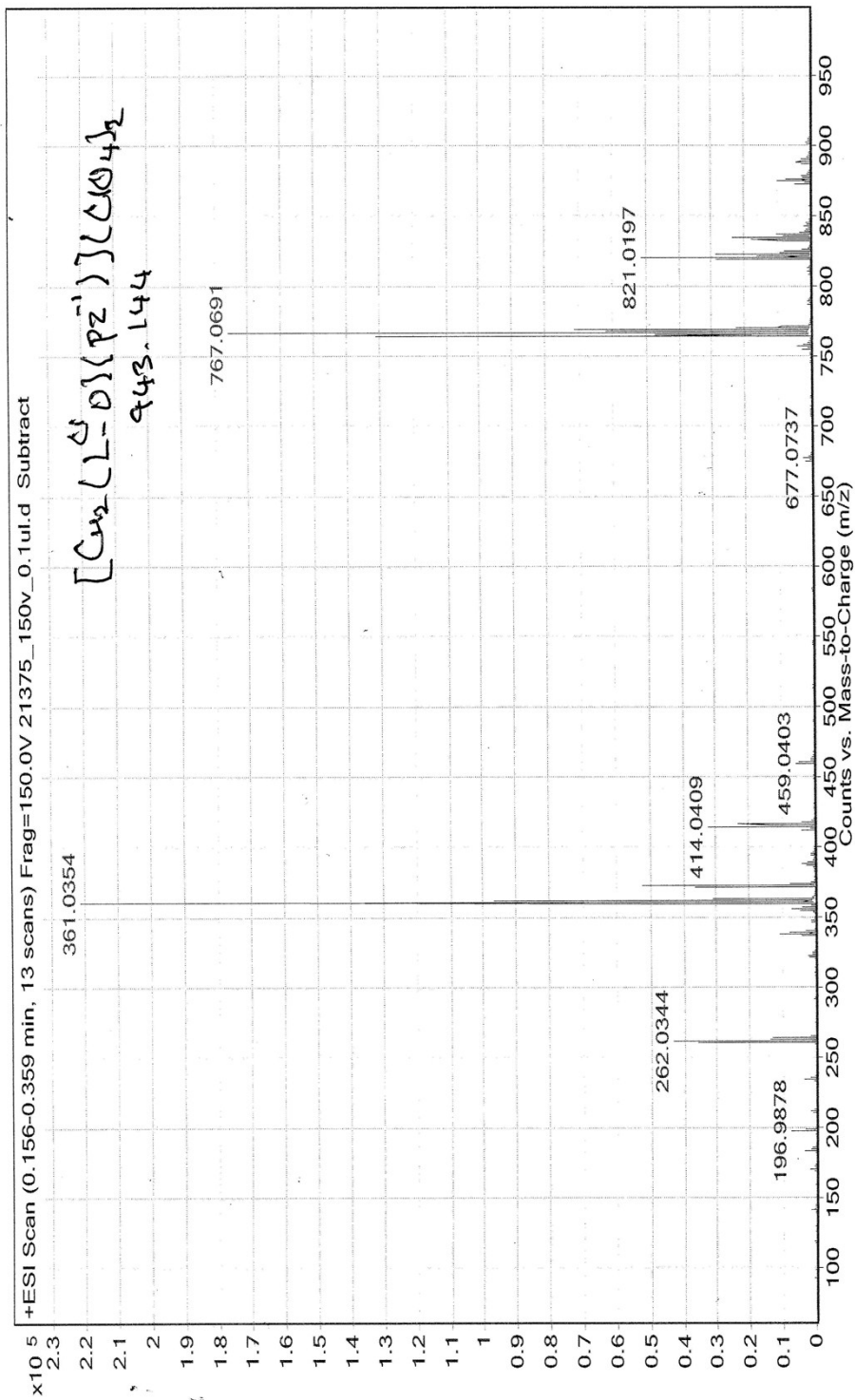


Fig. S2. ESI Mass spectrum of  $[Cu_2(\mu-L^{ClO})(\mu-C_3H_3N_2^-)](ClO_4)_2$  (**2**) in acetonitrile solution

881  
# 21376

#2746

pu

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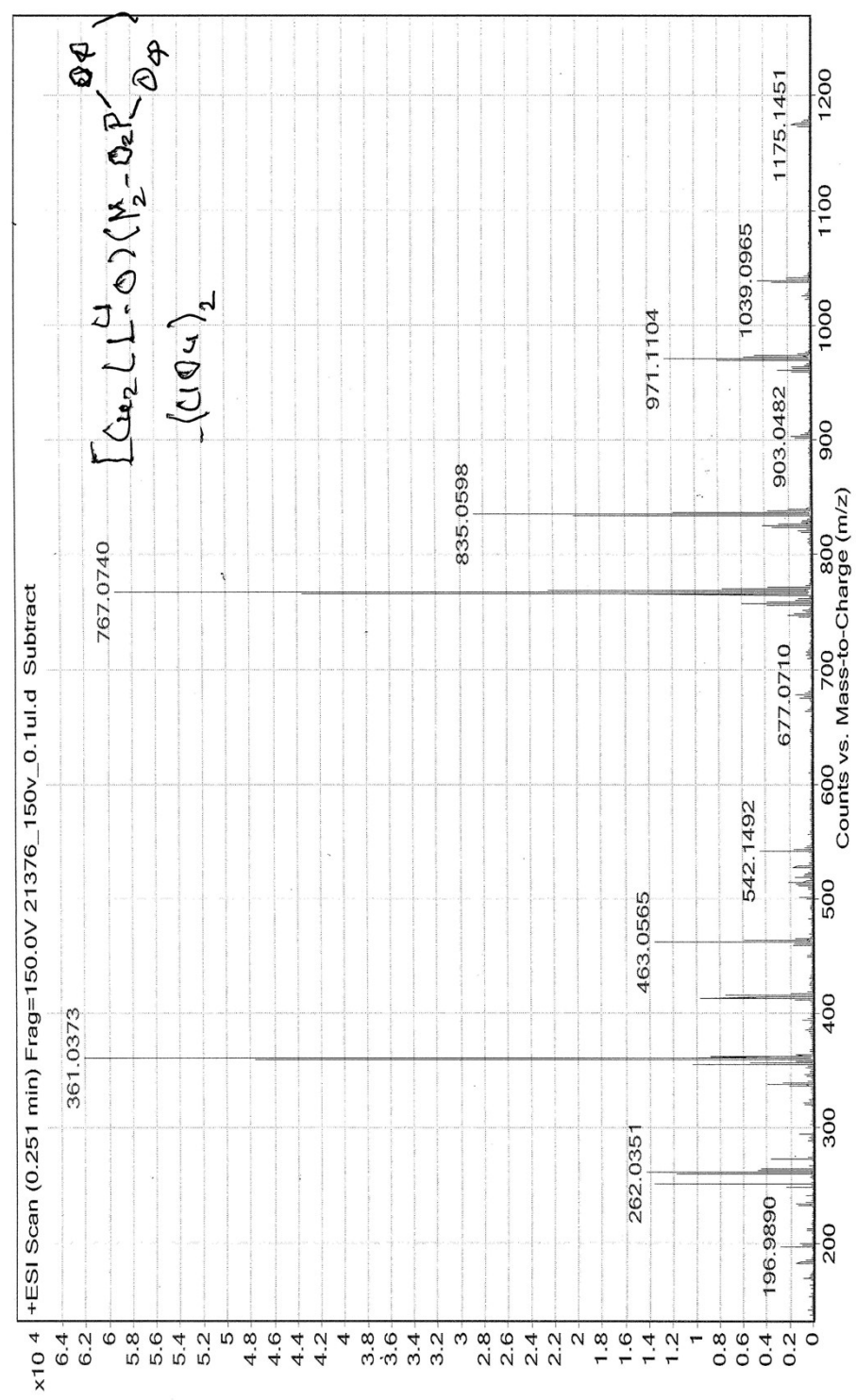


Fig. S3. ESI Mass spectrum of  $[Cu_2(L^{Cl-O})(\mu-O_2P(OC_6H_5)_2)(ClO_4)_2]$  (**3**) in acetonitrile solution

ESV  
# 2724

green soln  
L-O/dca/Cu<sup>2+</sup>/PF<sub>6</sub><sup>-</sup> # 21482

New

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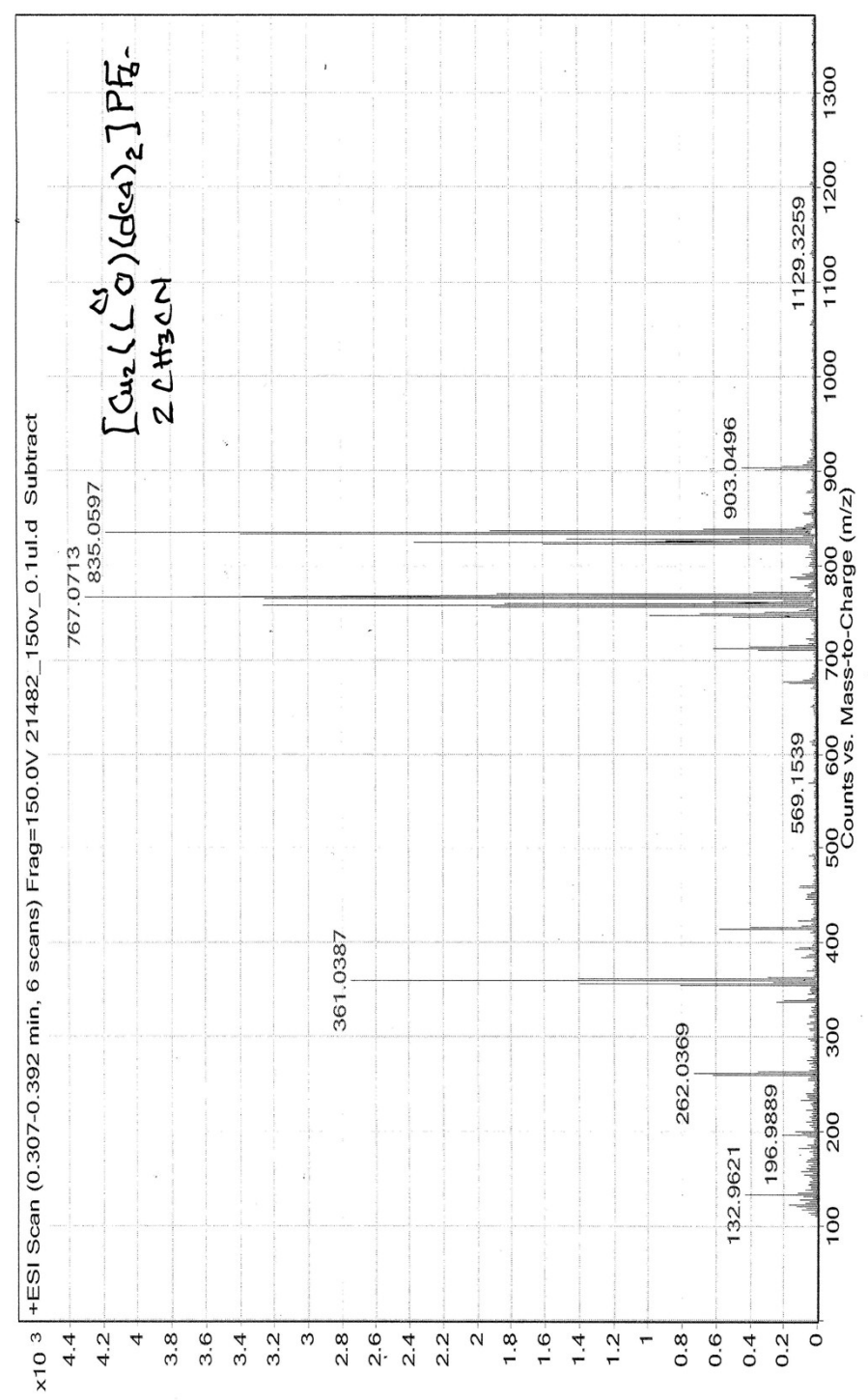
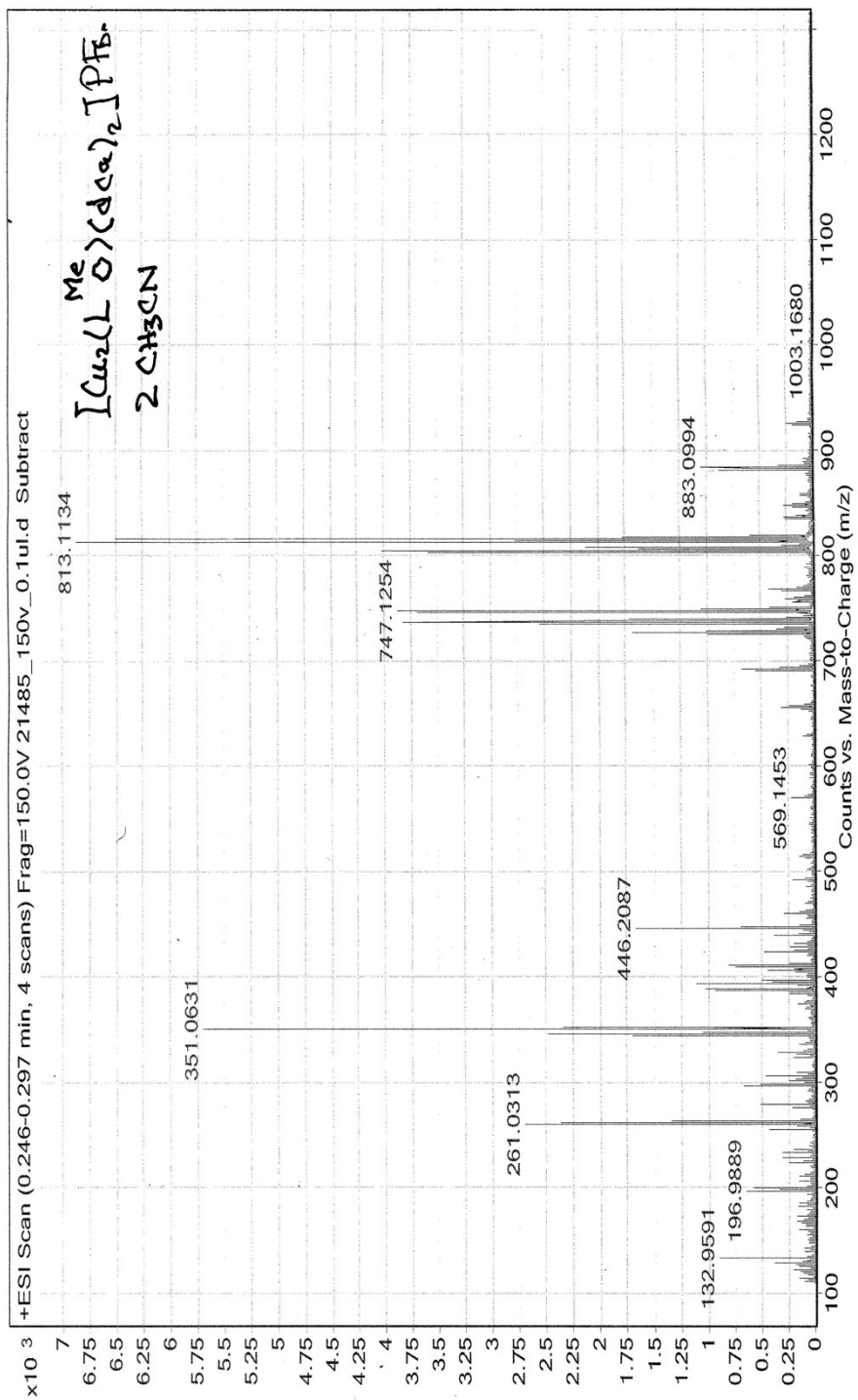
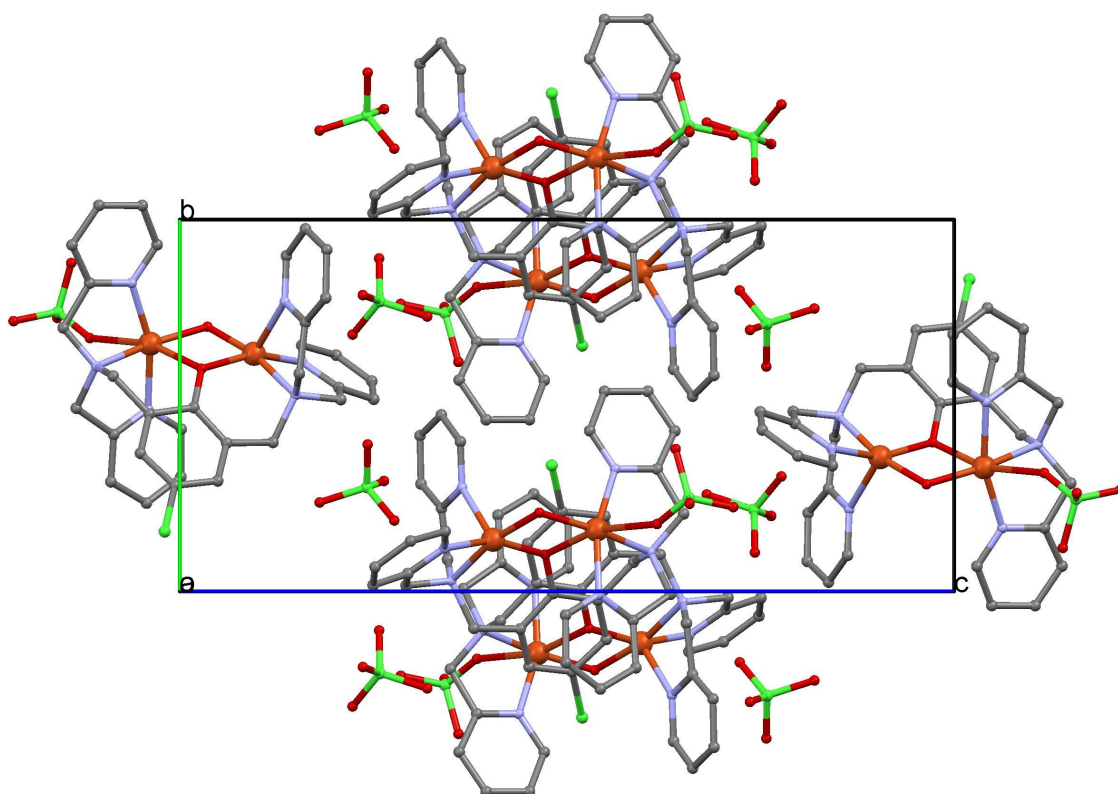


Fig. S4. ESI Mass spectrum of  $[Cu_2(\mu-L^{ClO})(dca)_2]PF_6 \cdot 2CH_3CN$  (4·2CH<sub>3</sub>CN) in acetonitrile solution

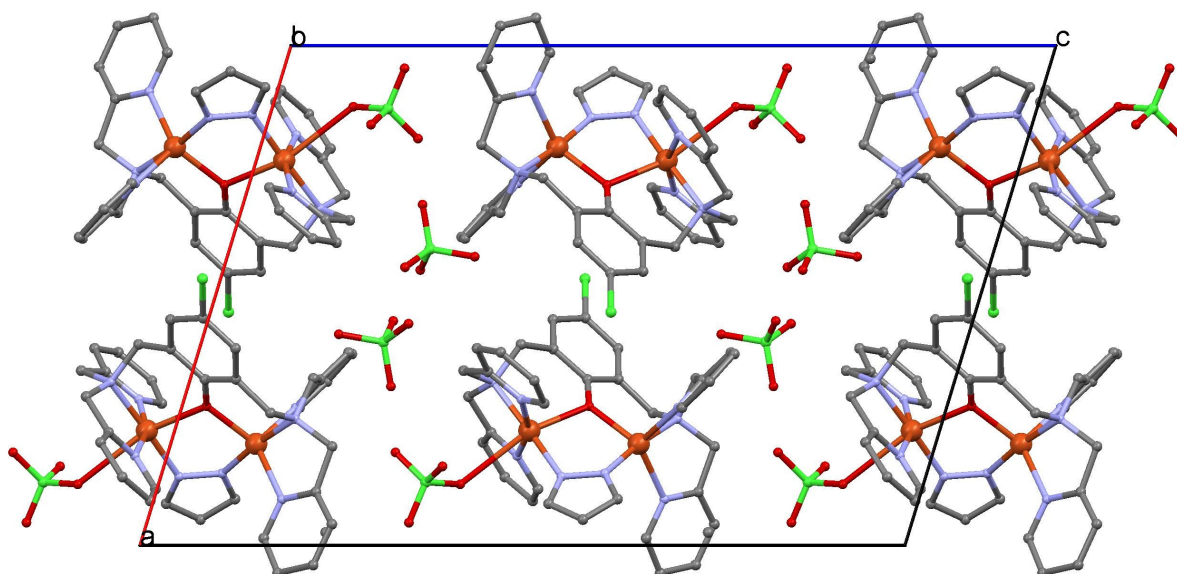
# 2648  
 # 21485  
 ESI  
 [Cu<sub>2</sub>(μ-L<sup>Me</sup>O)(dca)]PF<sub>6</sub>  
 New  
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 Position: Inj Position  
 Inj Vol: -1  
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 Instrument 1: Sample  
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 SUCCESS



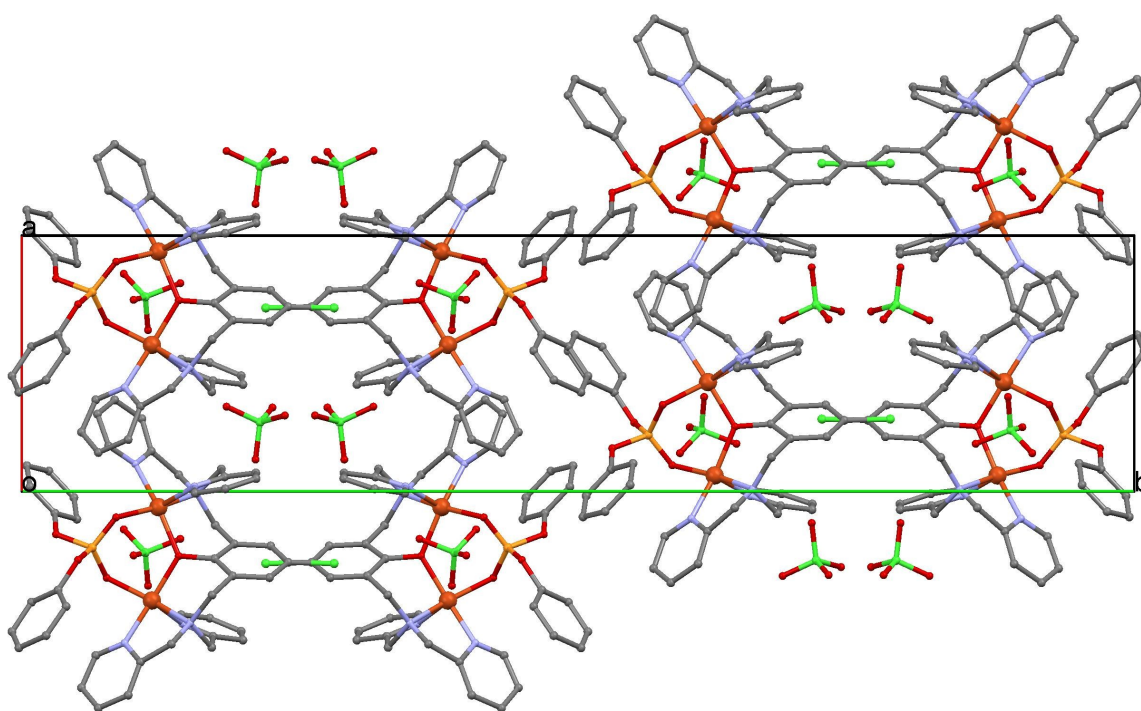
**Fig. S5.** ESI Mass spectrum of  $[Cu_2(\mu-L^{Me}O)(dca)_2]PF_6 \cdot 2CH_3CN$  (5·2CH<sub>3</sub>CN) in acetonitrile solution



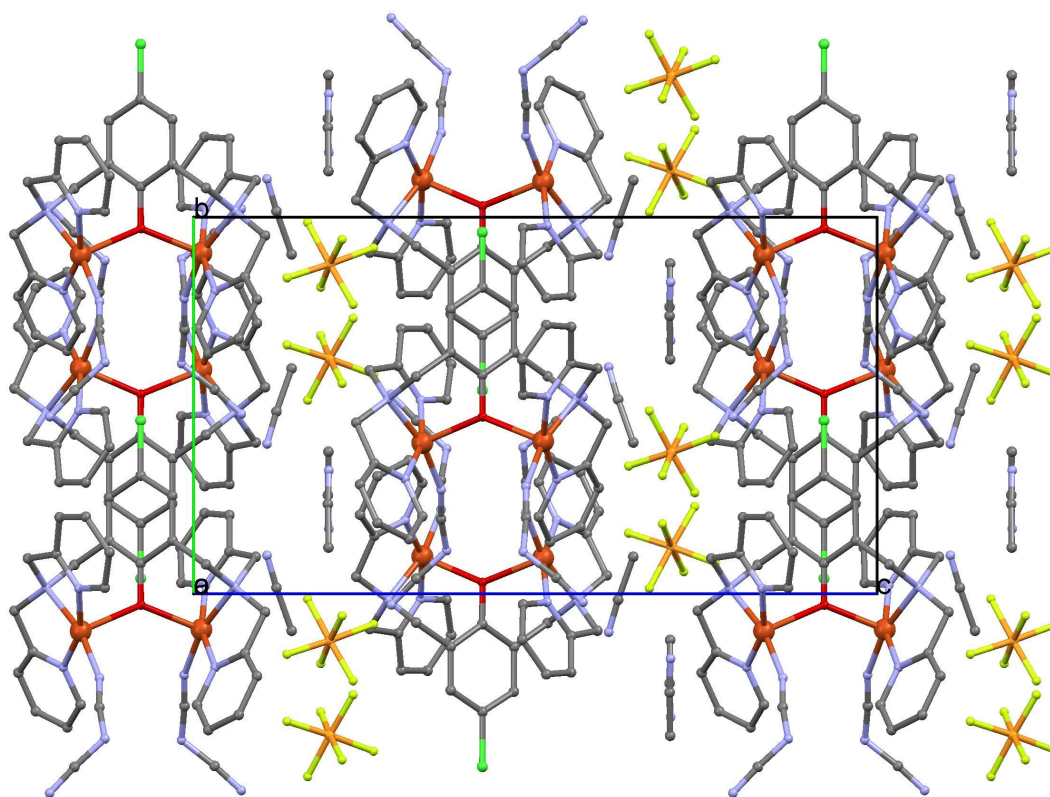
**Fig. S6.** Packing plot of 1



**Fig. S7.** Packing plot of 2

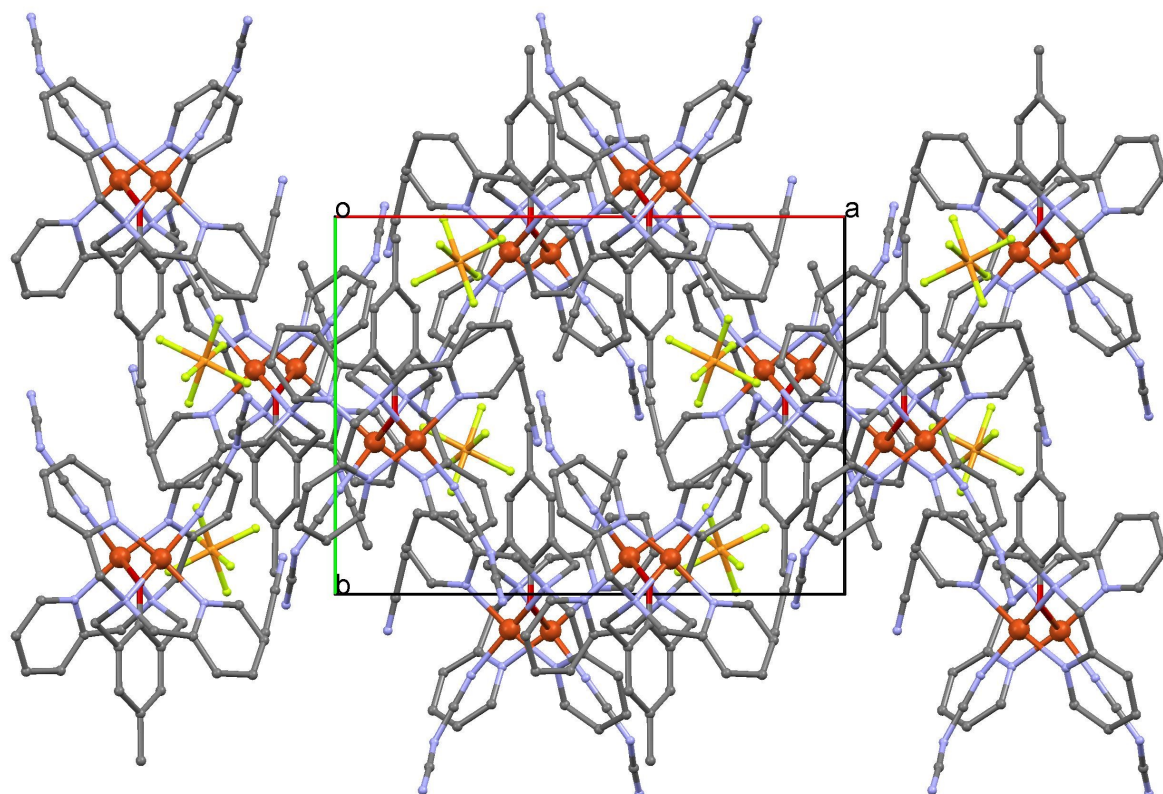


**Fig. S8.** Packing plot of **3**



**Fig. S9.** Packing plot of **4·2CH<sub>3</sub>CN**





**Fig. S10:** Packing plot of  $5 \cdot 2\text{CH}_3\text{CN}$

**Table S1** Selected bond distances (Å) and angles (°) for **1**

Cu(1)-N(2)	1.998(4)	Cu(1)-N(3)	2.205(5)
Cu(1)-N(1)	2.044(2)	Cu(1)-O(1)	1.959(3)
Cu(1)-O(10)	1.932(4)	Cu(2)-N(5)	1.988(5)
Cu(2)-N(6)	2.026(5)	Cu(2)-N(4)	2.041(4)
Cu(2)-O(1)	2.200(4)	Cu(2)-O(10)	1.932(3)
N(1)-Cu(1)-O(10)	168.05(19)	N(5)-Cu(2)-N(6)	162.48(17)
N(2)-Cu(1)-O(1)	159.0(2)	N(4)-Cu(2)-O(10)	170.71(17)
O(1)-Cu(2)-O(1)	78.27(14)	Cu(1)-O(10)-Cu(2)	103.29(18)
Cu(1)-O(1)-Cu(2)	93.36(15)		

**Table S2** Selected bond distances (Å) and angles (°) for **2**

Cu(1)-N(2)	2.020(6)	Cu(1)-N(3)	1.999(5)
Cu(1)-N(1)	2.015(4)	Cu(1)-O(1)	2.227(4)
Cu(1)-N(7)	1.957(5)	Cu(1)-O(2)	2.769(7)
Cu(2)-N(6)	2.088(5)	Cu(2)-N(4)	2.020(6)
Cu(2)-O(1)	2.029(4)	Cu(2)-N(8)	1.944(7)
Cu(2)-N(5B)	1.997(10)	Cu(2)-N(5A)	2.186(11)
N(7)-N(8)	1.362(7)		
N(1)-Cu(1)-N(7)	173.5(2)	O(1)-Cu(1)-O(2)	167.87(17)
N(3)-Cu(1)-N(2)	161.09(19)	N(4)-Cu(2)-N(8)	174.1(2)
O(1)-Cu(2)-N(5B)	130.6(3)	O(1)-Cu(2)-N(5A)	127.4(3)
Cu(1)-O(1)-Cu(2)	108.85(18)		

**Table S3.** Selected bond distances (Å) and angles (°) for **3**

Cu(1)-N(2)	2.140(4)	Cu(1)-N(3)	2.015(4)
Cu(1)-N(1)	2.034(4)	Cu(1)-O(1)	1.986(3)
Cu(1)-O(10)	1.959(3)	Cu(2)-N(5)	2.173(4)
Cu(2)-N(6)	2.005(4)	Cu(2)-N(4)	2.054(4)
Cu(2)-O(1)	1.986(3)	Cu(2)-O(11)	1.993(3)
N(1)-Cu(1)-O(10)	170.17(16)	O(1)-Cu(2)-N(6)	170.07(17)
N(3)-Cu(1)-O(1)	164.48(17)	N(4)-Cu(2)-O(11)	160.56(16)
Cu(2)-O(11)-P(1)	120.1(2)	Cu(1)-O(10)-P(1)	124.1(2)
Cu(1)-O(1)-Cu(2)	126.90(17)		

**Table S4** Selected bond distances (Å) and angles (°) for 4·2CH<sub>3</sub>CN

Cu(1)-N(2)	1.980(5)	Cu(1)-N(3)	1.972(5)
Cu(1)-N(1)	2.058(6)	Cu(1)-O(1)	2.190(5)
Cu(1)-N(7)	1.972(6)	Cu(2)-N(5)	1.993(5)
Cu(2)-N(6)	2.000(5)	Cu(2)-N(4)	2.046(5)
Cu(2)-O(1)	2.190(5)	Cu(2)-N(10)	1.961(5)
N(7)-C(34)	1.160(8)	N(8)-C(34)	1.288(9)
N(9)-C(35)	1.165(11)	N(8)-C(35)	1.342(11)
N(10)-C(36)	1.174(8)	N(11)-C(36)	1.286(9)
N(12)-C(37)	1.159(10)	N(11)-C(37)	1.324(10)
N(1)-Cu(1)-N(7)	165.2(3)	N(5)-Cu(2)-N(6)	161.3(3)
N(3)-Cu(1)-N(2)	162.1(3)	N(4)-Cu(2)-N(10)	165.2(3)
Cu(1)-N(7)-C(34)	161.0(6)	Cu(2)-N(10)-C(36)	162.1(6)
N(7)-C(34)-N(8)	175.0(9)	N(10)-C(36)-N(11)	172.0(8)
N(8)-C(35)-N(9)	173.8(8)	N(12)-C(37)-N(11)	174.2(7)
C(36)-N(11)-C(37)	117.8(7)	C(34)-N(8)-C(35)	119.8(7)
Cu(1)-O(1)-Cu(2)	136.82(17)		

**Table S5** Selected bond distances (Å) and angles (°) for 5·2CH<sub>3</sub>CN

Cu(1)-N(2)	1.989(2)	Cu(1)-N(3)	1.999(2)
Cu(1)-N(1)	2.045(2)	Cu(1)-O(1)	2.170(2)
Cu(1)-N(7)	1.962(3)	Cu(2)-N(5)	1.983(2)
Cu(2)-N(6)	1.982(2)	Cu(2)-N(4)	2.046(2)
Cu(2)-O(1)	2.172(2)	Cu(2)-N(10)	1.979(3)
N(7)-C(34)	1.161(4)	N(8)-C(34)	1.320(4)
N(9)-C(35)	1.142(4)	N(8)-C(35)	1.320(4)
N(10)-C(36)	1.153(4)	N(11)-C(36)	1.292(4)
N(12)-C(37)	1.154(4)	N(11)-C(37)	1.335(4)
N(1)-Cu(1)-N(7)	164.33(10)	N(5)-Cu(2)-N(6)	161.79(10)
N(3)-Cu(1)-N(2)	161.29(10)	N(4)-Cu(2)-N(10)	164.32(10)
Cu(1)-N(7)-C(34)	164.7(3)	Cu(2)-N(10)-C(36)	160.8(3)
N(7)-C(34)-N(8)	173.5(3)	N(10)-C(36)-N(11)	174.4(4)
N(8)-C(35)-N(9)	174.0(3)	N(12)-C(37)-N(11)	174.1(4)
C(36)-N(11)-C(37)	119.9(3)	C(34)-N(8)-C(35)	118.5(3)
Cu(1)-O(1)-Cu(2)	137.65(8)		