Supporting Information

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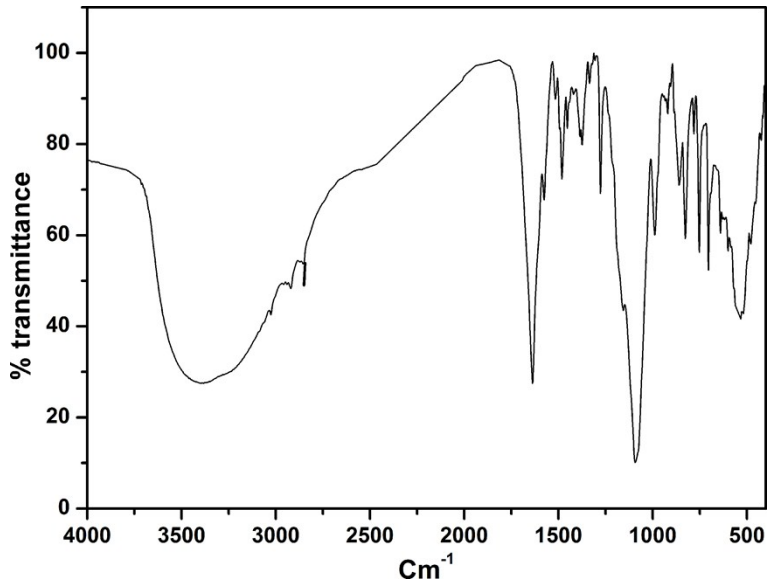
S1 Table Selected bond lengths (Å) and bond angles (°) for complexes 1 and 2.

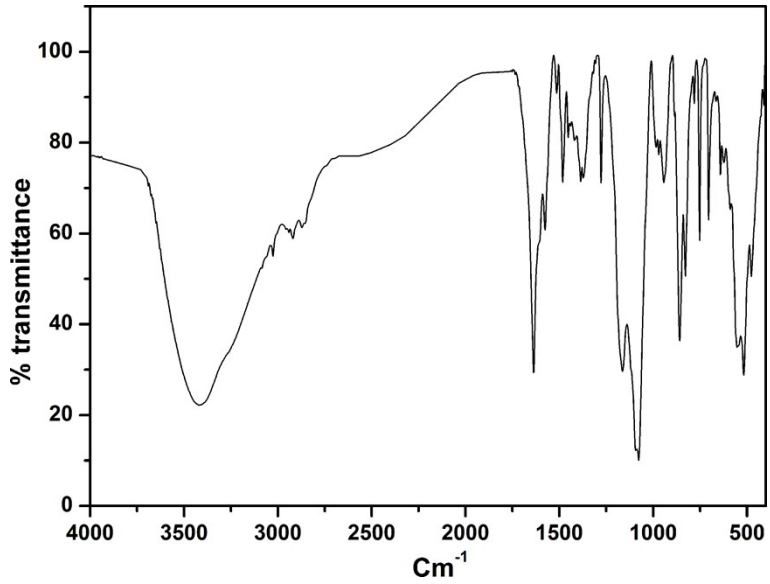
Complex 1			
Cu(1)-N(1)	1.84(2)	Cu(1)-O(9)	2.735(16)
Cu(4)-O(11)	2.756(19)	Cu(2)-O(23)	2.580(18)
Cu(5)-N(5)	1.91(2)	Cu(5)-O(18)	2.80(2)
Cu(3)-N(3)	1.956(19)	Cu(6)-N(6)	1.97(3)
Cu(8)-O(16)	1.78(2)	Cu(7)-O(18)	1.99(2)
Cu(4)-O(9)	1.911(15)	Cu(3)-O(9)	1.964(16)
Cu(2)-O(4)	2.556(15)	Cu(8)-O(18)	1.892(19)
O(3)-Cu(1)-O(1)	171.3(7)	O(6)-Cu(2)-O(5)	175.8(7)
O(13)-Cu(5)-N(5)	169.8(12)	O(13)-Cu(5)-O(18)	66.6(8)
O(4)-Cu(3)-O(9)	90.5(6)	O(17)-Cu(7)-O(13)	176.9(9)
N(2)-Cu(2)-O(6)	93.6(7)	N(1)-Cu(1)-O(1)	92.8(8)
Cu(4)-O(9)-Cu(1)	99.0(6)	O(5)-Cu(4)-O(3)	69.6(5)
Complex 2			
O(2)-Cu(1)	1.893(10)	O(5)-Cu(1)	2.832(16)
O(4)-Cu(1)#1	1.908(11)	O(1)-Cu(1)	1.929(12)
Cu(1)-N(1)	1.873(13)	Cu(1)-O(4)#1	1.908(11)
O(6)-Cu(2)	2.534(17)	Cu(2)-O(4)	1.934(10)
Cu(2)-O(3)	1.886(11)	Cu(2)-O(2)	1.967(11)
Cu(2)-N(2)	1.938(12)	N(2)-C(26)	1.485(19)
N(1)-C(7)	1.340(13)	N(1)-C(8)	1.41(2)
N(2)-C(25)	1.335(18)	N(2)-C(26)	1.485(19)
C(18)-O(5)-Cu(1)	129.6(16)	C(35)-O(6)-Cu(2)	132.8(18)
N(1)-Cu(1)-O(4)#1	166.3(6)	N(1)-Cu(1)-O(1)	95.9(7)
O(4)#1-Cu(1)-O(2)	87.5(5)	O(3)-Cu(2)-O(4)	174.1(5)
O(4)-Cu(2)-N(2)	82.5(5)	N(2)-Cu(2)-O(6)	90.1(5)
N(2)-Cu(2)-O(2)	169.6(5)	O(3)-Cu(2)-O(6)	100.9(6)

S2 Table H-Bonding Parameters for complexes 1 and 2.

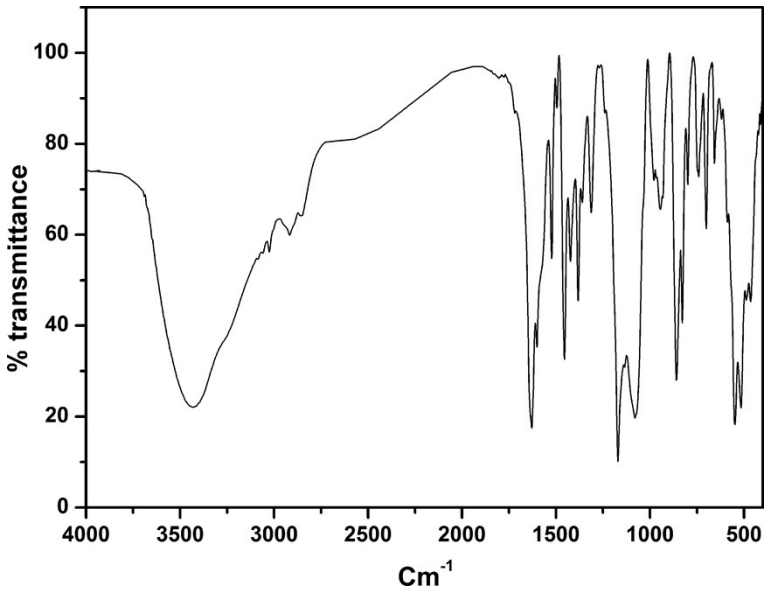
H-bonding	D---H(Å)	H---A(Å)	D---A(Å)	α (°)
Complex 1				
O(2)H(2)---O(6)	0.82	2.00	2.813	172.8
O(11)H(11)---O(7)	0.82	2.00	2.792	162.1
O(19)H(19)---O(12)	0.82	2.00	2.763	154.6
O(21)H(21C)---O(17)	0.82	1.96	2.768	167.0
O(22)H(22)---O(1)	0.82	2.04	2.845	168.0
O(23)H(23)---O(10)	0.82	2.08	2.862	158.8
O(24)H(24)---O(15)	0.82	2.02	2.818	164.5
O(25)H(25)---O(20)	0.82	2.01	2.822	169.5
C(16)H(16B)---Cl(7)#1	0.97	2.97	3.618	125.7
C(16)H(16B)---O(6)	0.97	2.46	2.998	114.4
C(32)H(32A)---O(23)	0.97	2.66	3.26	120.9
C(32)H(32B)---O(11)	0.97	2.61	3.32	129.6
C(48)H(48A)---O(22)	0.97	2.50	3.11	120.3
C(48)H(48B)---O(2)	0.97	2.59	3.25	125.8
C(56)H(56B)---Cl(2) #2	0.97	2.89	3.538	125.6
C(56)H(56B)---O(7)	0.97	2.43	3.006	117.9
C(65)H(65B)---Cl(3) #3	0.97	2.97	3.73	135.9
C(65)H(65B)---O(15)	0.97	2.53	3.10	118.0
C(88)H(88A)---O(25)	0.97	2.48	3.05	117.2
C(88)H(88B)---O(21)	0.97	2.46	3.17	129.3
C(97)H(97A)---O(19)	0.97	2.62	3.25	122.5
C(97)H(97B)---O(24)	0.97	2.52	3.24	131.2
C(113)H(11B)---O(17)	0.97	2.58	3.07	111.2
Complex 2				
O(5)H(5C)---O(3)	0.87	2.00	2.800	153.1
O(6)H(6C)---O(1)#4	0.89	2.15	2.889	139.7
O(16)H(16A)---O(3)	0.97	2.62	3.132	113.1
O(34)H(34A)---O(5)#4	0.97	2.37	3.139	136.2
O(34)H(34B)---O(6)	0.97	2.44	3.078	122.8
Symmetry codes: #1 x-1, y, z; #2 x, y-1, z; #3 x, y+1, z+1; #4 -x, y, -z				



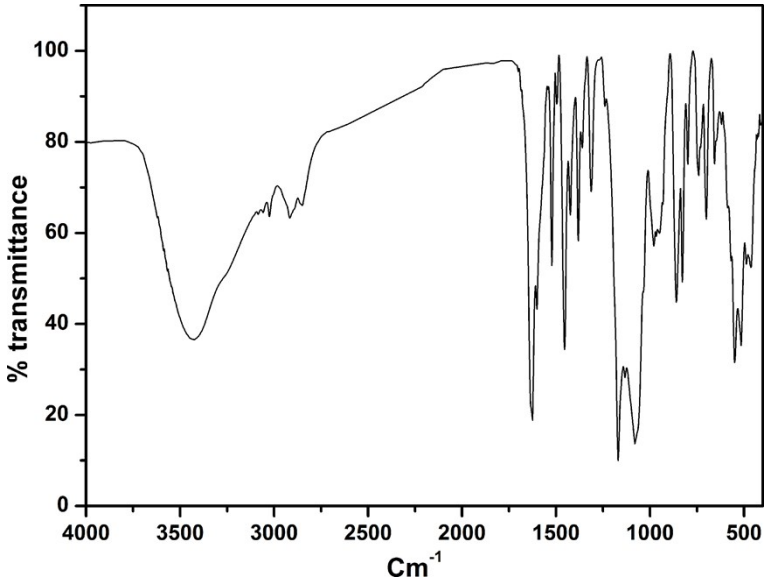
S1 Fig. IR spectrum of *R*-H_2L.



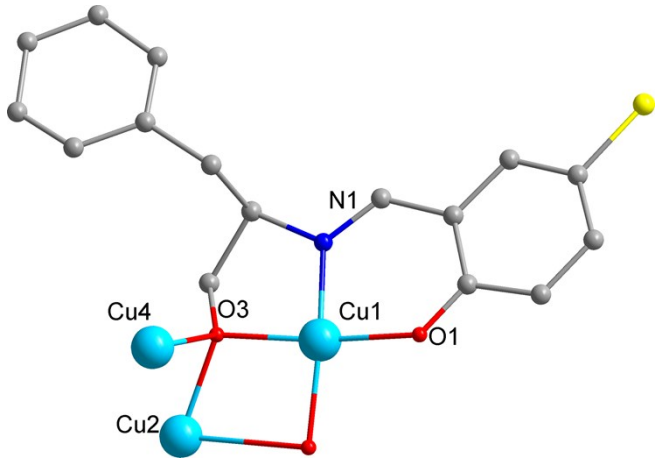
S2 Fig. IR spectrum of *S*-H_2L.



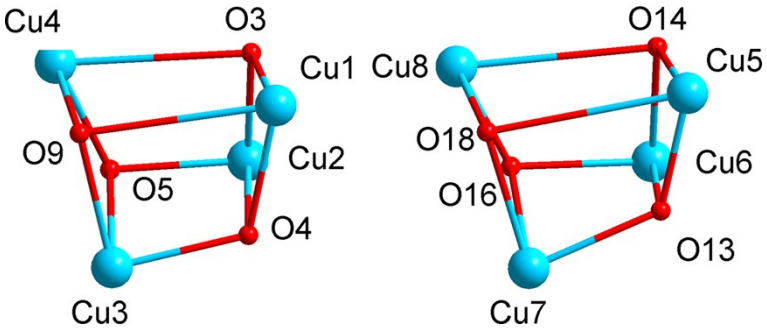
S3 Fig. IR spectrum of Cu(II) complex 1.



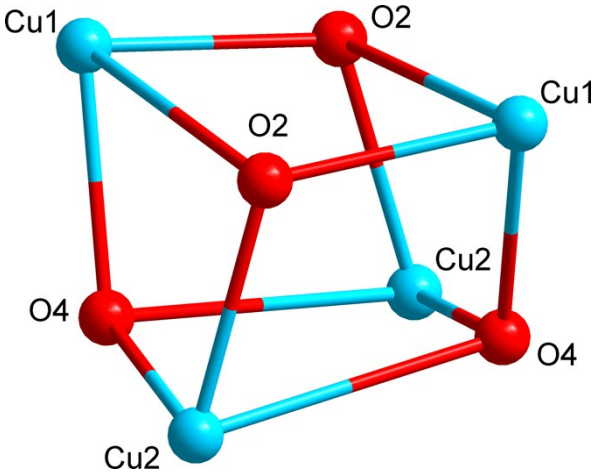
S4 Fig. IR spectrum of Cu(II) complex 2.



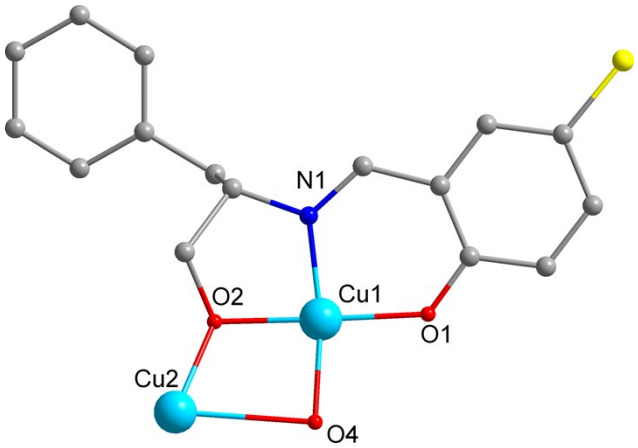
S5 Fig. The coordination mode of {(*R*)-L}$^{2-}$ in the complex 1.



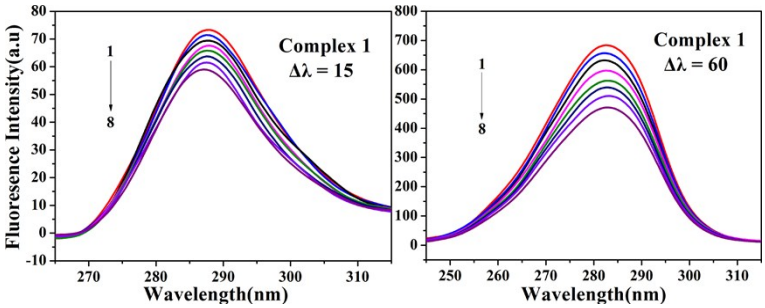
S6 Fig. The cubane - shaped $\{Cu_4O_4\}$ unit complex 1.



S7 Fig. The cubane - shaped $\{Cu_4O_4\}$ unit complex 2.



S8 Fig. The coordination mode of $\{(S)\text{-}L\}^{2-}$ in the complex 2.



S9 Fig. Synchronous spectra of BSA as a function of concentration of the complex 1 with wavelength difference of Δλ = 15 nm and Δλ = 60 nm.