

Supporting information

**Homochiral Coordination Cages Assembled from Dinuclear Paddlewheel Nodes and
Enantiopure Dipotic Ligands: Syntheses, Structures and Catalysis**

Lianfen Chen, Jian Kang, Hao Cui, Yingxia Wang, Lan Liu, Li Zhang,* and Cheng-Yong Su*

MOE Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional Materials,
School of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou 510275,
China.

Fax: (+86) 20-8411-5178

E-mail: zhli99@mail.sysu.edu.cn; cesscy@mail.sysu.edu.cn

Table S1 Selected bond lengths (Å) and bond Angles (°) for **1-4**

1			
Cu(1)-O(10)	1.959(5)	Cu(3)-O(2)#1	1.918(3)
Cu(1)-O(10)#1	1.959(5)	Cu(3)-O(2)	1.918(3)
Cu(1)-O(8)#1	2.001(3)	Cu(3)-O(16)#1	1.924(4)
Cu(1)-O(8)	2.001(3)	Cu(3)-O(16)	1.924(4)
Cu(1)-O(17)	2.129(7)	Cu(3)-O(19B)	2.377(16)
Cu(1)-Cu(2)	2.5660(14)	Cu(3)-Cu(4)	2.5743(18)
Cu(2)-O(7)#1	1.923(3)	Cu(4)-O(15)#1	1.959(8)
Cu(2)-O(7)	1.923(3)	Cu(4)-O(15)	1.959(8)
Cu(2)-O(9)	1.941(3)	Cu(4)-O(1)#1	2.018(5)
Cu(2)-O(9)#1	1.941(3)	Cu(4)-O(1)	2.018(5)
Cu(2)-O(19A)	2.347(16)	Cu(4)-O(18)	2.088(11)
O(10)-Cu(1)-O(10)#1	166.0(3)	C(1)-O(2)-Cu(3)	118.1(4)
O(10)-Cu(1)-O(8)#1	90.78(16)	C(18)-O(7)-Cu(2)	120.2(3)
O(10)#1-Cu(1)-O(8)#1	87.45(17)	O(2)-Cu(3)-O(16)	90.88(18)
O(10)-Cu(1)-O(8)	87.45(17)	O(16)#1-Cu(3)-O(16)	168.0(3)
O(10)#1-Cu(1)-O(8)	90.78(16)	O(2)#1-Cu(3)-O(19B)	89.76(13)
O(8)#1-Cu(1)-O(8)	165.4(2)	O(2)-Cu(3)-O(19B)	89.76(13)
O(10)-Cu(1)-O(17)	97.02(13)	O(16)#1-Cu(3)-O(19B)	95.99(15)
O(10)#1-Cu(1)-O(17)	97.02(13)	O(16)-Cu(3)-O(19B)	95.99(15)
O(8)#1-Cu(1)-O(17)	97.29(11)	O(2)#1-Cu(3)-Cu(4)	90.24(13)
O(8)-Cu(1)-O(17)	97.29(11)	O(2)-Cu(3)-Cu(4)	90.24(13)
O(10)-Cu(1)-Cu(2)	82.98(13)	O(16)#1-Cu(3)-Cu(4)	84.01(15)
O(10)#1-Cu(1)-Cu(2)	82.98(13)	O(16)-Cu(3)-Cu(4)	84.01(15)
O(8)#1-Cu(1)-Cu(2)	82.71(11)	O(19B)-Cu(3)-Cu(4)	180.000(1)
O(8)-Cu(1)-Cu(2)	82.71(11)	O(15)#1-Cu(4)-O(15)	171.5(4)
O(17)-Cu(1)-Cu(2)	180	O(15)#1-Cu(4)-O(1)#1	90.0(3)
O(7)#1-Cu(2)-O(7)	174.2(2)	O(15)-Cu(4)-O(1)#1	88.6(3)
O(7)#1-Cu(2)-O(9)	90.43(14)	O(15)#1-Cu(4)-O(1)	88.6(3)
O(7)-Cu(2)-O(9)	89.30(14)	O(15)-Cu(4)-O(1)	90.0(3)
O(7)#1-Cu(2)-O(9)#1	89.30(14)	O(1)#1-Cu(4)-O(1)	161.1(3)
O(7)-Cu(2)-O(9)#1	90.43(14)	O(15)#1-Cu(4)-O(18)	94.2(2)
O(9)-Cu(2)-O(9)#1	174.7(3)	O(15)-Cu(4)-O(18)	94.2(2)
O(7)#1-Cu(2)-O(19A)	92.89(10)	O(1)#1-Cu(4)-O(18)	99.46(14)
O(7)-Cu(2)-O(19A)	92.89(10)	O(1)-Cu(4)-O(18)	99.46(14)
O(9)-Cu(2)-O(19A)	92.67(13)	O(15)#1-Cu(4)-Cu(3)	85.8(2)
O(9)#1-Cu(2)-O(19A)	92.67(13)	O(15)-Cu(4)-Cu(3)	85.8(2)
O(7)#1-Cu(2)-Cu(1)	87.11(10)	O(1)#1-Cu(4)-Cu(3)	80.54(14)
O(7)-Cu(2)-Cu(1)	87.11(10)	O(1)-Cu(4)-Cu(3)	80.54(14)
O(9)-Cu(2)-Cu(1)	87.33(13)	O(18)-Cu(4)-Cu(3)	180
O(9)#1-Cu(2)-Cu(1)	87.33(13)	C(1)-O(1)-Cu(4)	124.2(4)

Cu(1)-O(1)	1.975(11)	Cu(3)-O(13)#1	1.916(4)
Cu(1)-O(1)#1	1.975(11)	Cu(3)-O(13)	1.916(4)
Cu(1)-O(9)#1	2.011(6)	Cu(3)-O(6)#1	1.933(5)
Cu(1)-O(9)	2.011(6)	Cu(3)-O(6)	1.933(5)
Cu(1)-O(17)	2.074(14)	Cu(3)-O(19B)	2.38(2)
Cu(1)-Cu(2)	2.580(2)	Cu(3)-Cu(4)	2.5691(18)
Cu(2)-O(2)#1	1.914(6)	Cu(4)-O(5)#1	1.962(6)
Cu(2)-O(2)	1.914(6)	Cu(4)-O(5)	1.962(6)
Cu(2)-O(10)#1	1.917(5)	Cu(4)-O(14)#1	1.980(5)
Cu(2)-O(10)	1.917(5)	Cu(4)-O(14)	1.980(5)
		Cu(4)-O(18)	2.140(8)
O(1)-Cu(1)-O(1)#1	171.6(5)	O(13)-Cu(3)-O(6)#1	88.90(19)
O(1)-Cu(1)-O(9)#1	90.3(3)	O(13)#1-Cu(3)-O(6)	88.90(19)
O(1)#1-Cu(1)-O(9)#1	88.3(3)	O(13)-Cu(3)-O(6)	90.88(19)
O(1)-Cu(1)-O(9)	88.3(3)	O(6)#1-Cu(3)-O(6)	174.5(3)
O(1)#1-Cu(1)-O(9)	90.3(3)	O(13)#1-Cu(3)-O(19B)	92.28(14)
O(9)#1-Cu(1)-O(9)	161.7(4)	O(13)-Cu(3)-O(19B)	92.28(14)
O(1)-Cu(1)-O(17)	94.2(2)	O(6)#1-Cu(3)-O(19B)	92.74(16)
O(1)#1-Cu(1)-O(17)	94.2(2)	O(6)-Cu(3)-O(19B)	92.74(16)
O(9)#1-Cu(1)-O(17)	99.14(18)	O(13)#1-Cu(3)-Cu(4)	87.72(14)
O(9)-Cu(1)-O(17)	99.14(18)	O(13)-Cu(3)-Cu(4)	87.72(14)
O(1)-Cu(1)-Cu(2)	85.8(2)	O(6)#1-Cu(3)-Cu(4)	87.26(16)
O(1)#1-Cu(1)-Cu(2)	85.8(2)	O(6)-Cu(3)-Cu(4)	87.26(16)
O(9)#1-Cu(1)-Cu(2)	80.86(18)	O(19B)-Cu(3)-Cu(4)	180.0(8)
O(9)-Cu(1)-Cu(2)	80.86(18)	O(5)#1-Cu(4)-O(5)	165.4(4)
O(17)-Cu(1)-Cu(2)	180.0(7)	O(5)#1-Cu(4)-O(14)#1	90.3(2)
O(2)#1-Cu(2)-O(2)	168.1(4)	O(5)-Cu(4)-O(14)#1	87.7(2)
O(2)#1-Cu(2)-O(10)#1	89.3(2)	O(5)#1-Cu(4)-O(14)	87.7(2)
O(2)-Cu(2)-O(10)#1	90.8(2)	O(5)-Cu(4)-O(14)	90.3(2)
O(2)#1-Cu(2)-O(10)	90.8(2)	O(14)#1-Cu(4)-O(14)	164.7(3)
O(2)-Cu(2)-O(10)	89.3(2)	O(5)#1-Cu(4)-O(18)	97.28(18)
O(10)#1-Cu(2)-O(10)	179.7(4)	O(5)-Cu(4)-O(18)	97.28(18)
O(2)#1-Cu(2)-O(19A)	96.0(2)	O(14)#1-Cu(4)-O(18)	97.67(15)
O(2)-Cu(2)-O(19A)	96.0(2)	O(14)-Cu(4)-O(18)	97.67(15)
O(10)#1-Cu(2)-O(19A)	89.87(17)	O(5)#1-Cu(4)-Cu(3)	82.72(18)
O(10)-Cu(2)-O(19A)	89.87(17)	O(5)-Cu(4)-Cu(3)	82.72(18)
O(2)#1-Cu(2)-Cu(1)	84.0(2)	O(14)#1-Cu(4)-Cu(3)	82.33(15)
O(2)-Cu(2)-Cu(1)	84.0(2)	O(14)-Cu(4)-Cu(3)	82.33(15)
O(10)#1-Cu(2)-Cu(1)	90.13(17)	O(18)-Cu(4)-Cu(3)	180.00(11)
O(10)-Cu(2)-Cu(1)	90.13(17)	C(17)-O(1)-Cu(1)	117.2(7)
O(19A)-Cu(2)-Cu(1)	180.0(8)	C(17)-O(2)-Cu(2)	122.6(8)
O(13)#1-Cu(3)-O(13)	175.4(3)	C(8)-O(5)-Cu(4)	123.7(5)
O(13)#1-Cu(3)-O(6)#1	90.88(19)	C(8)-O(6)-Cu(3)	120.1(5)

C(36)-O(9)-Cu(1)	C(36)-O(9)-Cu(1)	C(19)-O(13)-Cu(3)	120.0(4)
C(36)-O(10)-Cu(2)	C(36)-O(10)-Cu(2)	C(19)-O(14)-Cu(4)	124.5(4)

3

Cu(1)-O(1)	1.9653(16)	Cu(2)-O(10)	1.9396(14)
Cu(1)-O(15)#1	1.9702(15)	Cu(2)-O(16)#1	1.9406(14)
Cu(1)-O(9)	1.9693(15)	Cu(2)-O(7)	1.9462(15)
Cu(1)-O(8)	1.9755(17)	O(1)-C(23)	1.256(3)
Cu(1)-N(5)	2.156(2)	O(2)-C(23)	1.258(3)
Cu(1)-Cu(2)	2.5743(4)	O(15)-Cu(1)#1	O(15)-Cu(1)#1
Cu(2)-O(2)	1.9389(15)	O(16)-C(22)	O(16)-C(22)
O(1)-Cu(1)-O(15)#1	89.67(6)	O(2)-Cu(2)-O(16)#1	90.64(6)
O(1)-Cu(1)-O(9)	88.90(7)	O(10)-Cu(2)-O(16)#1	172.60(7)
O(15)#1-Cu(1)-O(9)	167.99(7)	O(2)-Cu(2)-O(7)	175.51(7)
O(1)-Cu(1)-O(8)	164.91(7)	O(10)-Cu(2)-O(7)	89.05(6)
O(15)#1-Cu(1)-O(8)	89.77(7)	O(16)#1-Cu(2)-O(7)	89.88(6)
O(9)-Cu(1)-O(8)	88.52(7)	O(2)-Cu(2)-Cu(1)	85.62(5)
O(1)-Cu(1)-N(5)	106.02(7)	O(10)-Cu(2)-Cu(1)	85.41(5)
O(15)#1-Cu(1)-N(5)	94.63(7)	O(16)#1-Cu(2)-Cu(1)	87.26(5)
O(9)-Cu(1)-N(5)	97.23(7)	O(7)-Cu(2)-Cu(1)	89.94(5)
O(8)-Cu(1)-N(5)	89.06(7)	C(23)-O(1)-Cu(1)	121.23(15)
O(1)-Cu(1)-Cu(2)	84.69(5)	C(23)-O(2)-Cu(2)	121.39(14)
O(15)#1-Cu(1)-Cu(2)	83.19(5)	C(20)-O(7)-Cu(2)	116.39(15)
O(9)-Cu(1)-Cu(2)	84.80(5)	C(20)-O(8)-Cu(1)	126.37(15)
O(8)-Cu(1)-Cu(2)	80.27(5)	C(1)-O(9)-Cu(1)	121.14(14)
N(5)-Cu(1)-Cu(2)	169.10(6)	C(1)-O(10)-Cu(2)	121.73(14)
O(2)-Cu(2)-O(10)	89.87(6)	C(22)-O(15)-Cu(1)#1	123.03(15)
		C(22)-O(16)-Cu(2)#1	119.75(14)

4

O(1)-Cu(1)	1.9888	O(58)-Cu(7)	1.9539
O(2)-Cu(2)	1.9159	O(59)-Cu(8)	1.9676
O(3)-Cu(2)	1.9516	O(60)-Cu(7)	1.9149
O(4)-Cu(1)	1.9473	O(65)-Cu(5)	1.9777
O(5)-Cu(1)	1.9654	O(66)-Cu(6)	1.9342
O(6)-Cu(2)	1.9416	O(67)-Cu(5)	2.1051
O(7)-Cu(1)	1.9738	O(68)-Cu(8)	2.1696
O(8)-Cu(2)	1.9412	Cu(5)-Cu(6)	2.5631
O(13)-Cu(4)	1.9611	Cu(7)-Cu(8)	2.5656
O(15)-Cu(4)	1.9745	O(70)-Cu(10)	1.9415
O(16)-Cu(3)	1.9601	O(75)-Cu(11)	1.9463
O(17)-Cu(4)	1.9539	O(76)-Cu(12)	1.9361
O(18)-Cu(3)	1.9566	O(77)-Cu(12)	1.9831
O(19)-Cu(4)	1.9633	O(78)-Cu(11)	1.9404
O(20)-Cu(3)	1.9264	O(91)-Cu(9)	1.9722

O(33)-Cu(1)	2.1212	O(92)-Cu(10)	1.9271
O(34)-Cu(4)	2.1194	O(93)-Cu(9)	1.963
Cu(1)-Cu(2)	2.5694	O(94)-Cu(10)	1.9398
Cu(3)-Cu(4)	2.567	O(95)-Cu(9)	1.964
O(35)-Cu(5)	1.9381	O(96)-Cu(10)	1.9194
O(36)-Cu(6)	1.9372	O(97)-Cu(12)	1.9702
O(41)-Cu(8)	1.935	O(98)-Cu(11)	1.9389
O(42)-Cu(7)	1.9573	O(99)-Cu(11)	1.9476
O(43)-Cu(8)	1.9684	O(100)-Cu(12)	1.9505
O(44)-Cu(7)	1.92	O(101)-Cu(12)	2.1415
O(49)-Cu(5)	1.969	(102)-Cu(9)	2.1311
O(50)-Cu(6)	1.9411	Cu(9)-Cu(10)	2.5658
O(51)-Cu(5)	1.9653	Cu(11)-Cu(12)	2.5652
O(52)-Cu(6)	1.9494	O(69)-Cu(9)	1.9587
O(57)-Cu(8)	1.9418		
C(273)-O(1)-Cu(1)	122.9	C(197)-O(35) -Cu(5)	125.1
C(273)-O(2)-Cu(2)	122.3	C(197)-O(36) -Cu(6)	119.2
C(274)-O(3)-Cu(2)	118.6	C(173)-O(41) -Cu(8)	122.5
C(274)-O(4)-Cu(1)	126.4	C(173)-O(42) -Cu(7)	121.3
C(226)-O(5)-Cu(1)	119.3	C(125)-O(43) -Cu(8)	123.4
C(226)-O(6)-Cu(2)	123.6	C(125)-O(44) -Cu(7)	120.4
C(225)-O(7)-Cu(1)	126.6	C(148)-O(49) -Cu(5)	126.3
C(225)-O(8)-Cu(2)	117.4	C(148)-O(50) -Cu(6)	117.2
C(249)-O(13)-Cu(4)	122	C(101)-O(51) -Cu(5)	123.6
C(249)-O(14)-Cu(3)	121.7	C(101)-O(52) -Cu(6)	121.5
C(250)-O(15)-Cu(4)	124.5	C(120)-O(57) -Cu(8)	124.3
C(250)-O(16)-Cu(3)	117.8	C(120)-O(58) -Cu(7)	118.4
C(293)-O(17)-Cu(4)	124.2	C(172)-O(59) -Cu(8)	123.4
C(293)-O(18)-Cu(3)	118.3	C(172)-O(60) -Cu(7)	122.1
C(202)-O(19)-Cu(4)	121.3	C(149)-O(65) -Cu(5)	121.6
C(202)-O(20)-Cu(3)	121.9	C(149)-O(66) -Cu(6)	120.9
C(300)-O(33)-Cu(1)	127.7	C(198)-O(67) -Cu(5)	127.2
C(298)-O(34)-Cu(4)	125.9	C(199)-O(68) -Cu(8)	125.6
O(1)-Cu(1)-O(33)	99.7	O(35)-Cu(5) -O(49)	89
O(1)-Cu(1)-Cu(2)	83.3	O(35)-Cu(5) -O(51)	166.8
O(4)-Cu(1)O(1)	88.9	O(35)-Cu(5) -O(65)	89.3
O(4)-Cu(1)-O(5)	168.5	O(35)-Cu(5) -O(67)	95.7
O(4)-Cu(1)-O(7)	88.6	O(35)-Cu(5) -Cu(6)	83
O(4)-Cu(1)-O(33)	94	O(49)-Cu(5) -O(65)	165
O(4)-Cu(1)-Cu(2)	82.1	O(49)-Cu(5) -O(67)	94.2
O(5)-Cu(1)-O(1)	89.2	O(49)-Cu(5)- Cu(6)	80.9
O(5)-Cu(1)-O(7)	90	O(51)-Cu(5) -O(49)	88.4
O(5)-Cu(1)-O(33)	97.5	O(51)-Cu(5) -O(65)	89.8

O(5)-Cu(1)-Cu(2)	86.4	O(51)-Cu(5) -O(67)	97.4
O(7)-Cu(1)-O(1)	163.8	O(51)-Cu(5) -Cu(6)	83.8
O(7)-Cu(1)-O(33)	96.5	O(65)-Cu(5) -O(67)	100.9
O(7)-Cu(1)-Cu(2)	80.5	O(65)-Cu(5) -Cu(6)	84.1
O(33)-Cu(1)-Cu(2)	175.1	O(67)-Cu(5) -Cu(6)	174.9
O(2)-Cu(2)-O(3)	89.5	O(36)-Cu(6) -O(50)	89
O(2)-Cu(2)-O(6)	91.1	O(36)-Cu(6) -O(52)	174
O(2)-Cu(2)-O(8)	176.9	O(36)-Cu(6) -Cu(5)	87.9
O(2)-Cu(2)-Cu(1)	86.7	O(50)-Cu(6)-O(52)	89.1
O(3)-Cu(2)-Cu(1)	88.1	C(72)-O(69) -Cu(9)	124.5
O(6)-Cu(2)-O(3)	172	C(72)-O(70) -Cu(10)	120
O(6)-Cu(2)-Cu(1)	84	C(49)-O(75) -Cu(11)	119.1
O(8)-Cu(2)-O(3)	89.7	C(49)-O(76) -Cu(12)	122.9
O(8)-Cu(2)-O(6)	89.3	C(96)-O(77) -Cu(12)	122.3
O(8)-Cu(2)-Cu(1)	90.2	C(96)-O(78) -Cu(11)	119.7
O(14)-Cu(3)-O(16)	90	C(25)- O(91)- Cu(9)	122
O(14)-Cu(3)-O(18)	173.7	C(25)-O(92) -Cu(10)	120.5
O(14)-Cu(3)-Cu(4)	86	C(24)-O(93) -Cu(9)	122.4
O(16)-Cu(3)-Cu(4)	88.3	C(24)-O(94) -Cu(10)	122.2
O(18)-Cu(3)-O(16)	88.3	C(73)-O(95)- Cu(9)	125.8
O(18)-Cu(3)-Cu(4)	87.8	C(73)-O(96)-Cu(10)	119.3
O(20)-Cu(3)-O(14)	89.8	C(48)-O(97)-Cu(12)	123.7
O(20)-Cu(3)-O(16)	174.8	C(48)-O(98)-Cu(11)	117.6
O(20)-Cu(3)-O(18)	91.3	C(1)-O(99)-Cu(11)	120
O(20)-Cu(3)-Cu(4)	86.5	C(1)-O(100) -Cu(12)	126.8
O(13)-Cu(4)-O(15)	90.5	C(99)-O(101)-Cu(12)	120.4
O(13)-Cu(4)-O(19)	89.1	C(97)-O(102)-Cu(9)	125.3
O(13)-Cu(4)-O(34)	96.1	O(69)-Cu(9)-O(91)	90.4
O(13)-Cu(4)-Cu(3)	84.5	O(69)-Cu(9)-O(93)	167.4
O(15)-Cu(4)-O(34)	96.4	O(69)-Cu(9)-O(95)	87.6
O(15)-Cu(4)-Cu(3)	82.1	O(69)-Cu(9)-O(102)	93.5
O(17)-Cu(4)-O(13)	167.6	O(69)-Cu(9)-Cu(10)	83.1
O(17)-Cu(4)-O(15)	87.3	O(91)-Cu(9)-O(102)	96.6
O(17)-Cu(4)-O(19)	90.1	O(91)-Cu(9)-Cu(10)	82.9
O(17)-Cu(4)-O(34)	96.2	O(93)-Cu(9)-O(91)	88.6
O(17)-Cu(4)-Cu(3)	83.1	O(93)-Cu(9)-O(95)	90.1
O(19)-Cu(4)-O(15)	166.2	O(93)-Cu(9)-O(102)	99.1
O(19)-Cu(4)-O(34)	97.3	O(93)-Cu(9)-Cu(10)	84.4
O(19)-Cu(4)-Cu(3)	84.2	O(95)-Cu(9)-O(91)	164.7
O(34)-Cu(4)-Cu(3)	178.4	O(95)-Cu(9)-O(102)	98.6

Table S2 Asymmetric cyclopropanation catalyzed by cage compounds.

entry	Catalyst	Solvent	T/°C	ee (%) ^a
1	1	Acetone	40	3
2	3	Acetone	40	-1
3	4	Acetone	40	-6
4	1	TFT	40	N.D. ^b
5	3	TFT	40	16
6	4	TFT	40	-22
7	1	TFT	80	-6
8	3	TFT	80	13
9	4	TFT	80	-13

^aThe ee values were those of the *E*-cyclopropanes and determined by chiral HPLC analysis after purification (Daicel Chiralcel OJ column). ^bNot determined.

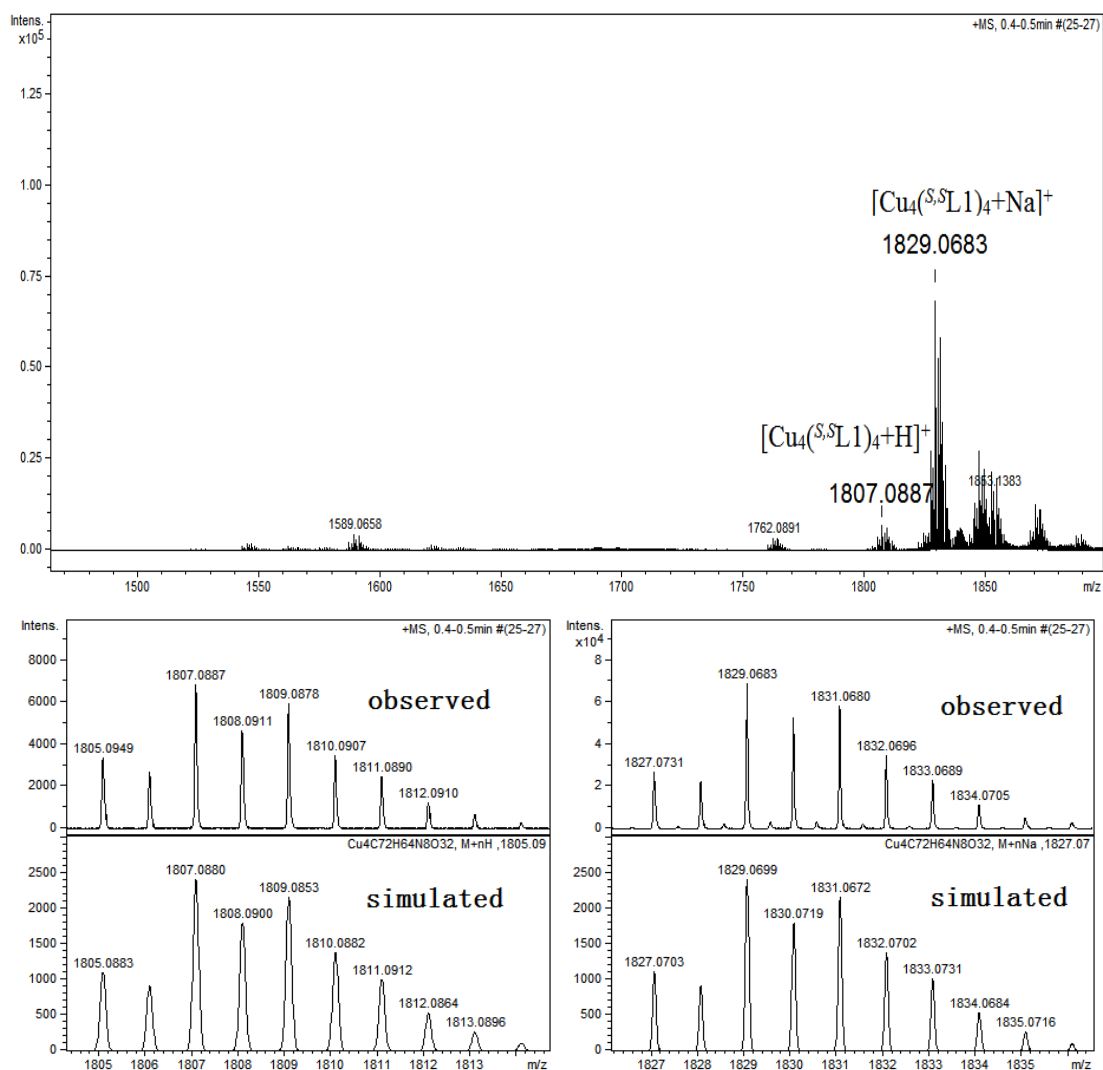


Figure S1a Partial HR-MS(ESI) of **1** in methanol (up). Isotopic distributions and simulations of the $[\text{Cu}_4\text{L}_4+\text{H}]^+$ (down left) and $[\text{Cu}_4\text{L}_4+\text{Na}]^+$ (down right) peaks are amplified.

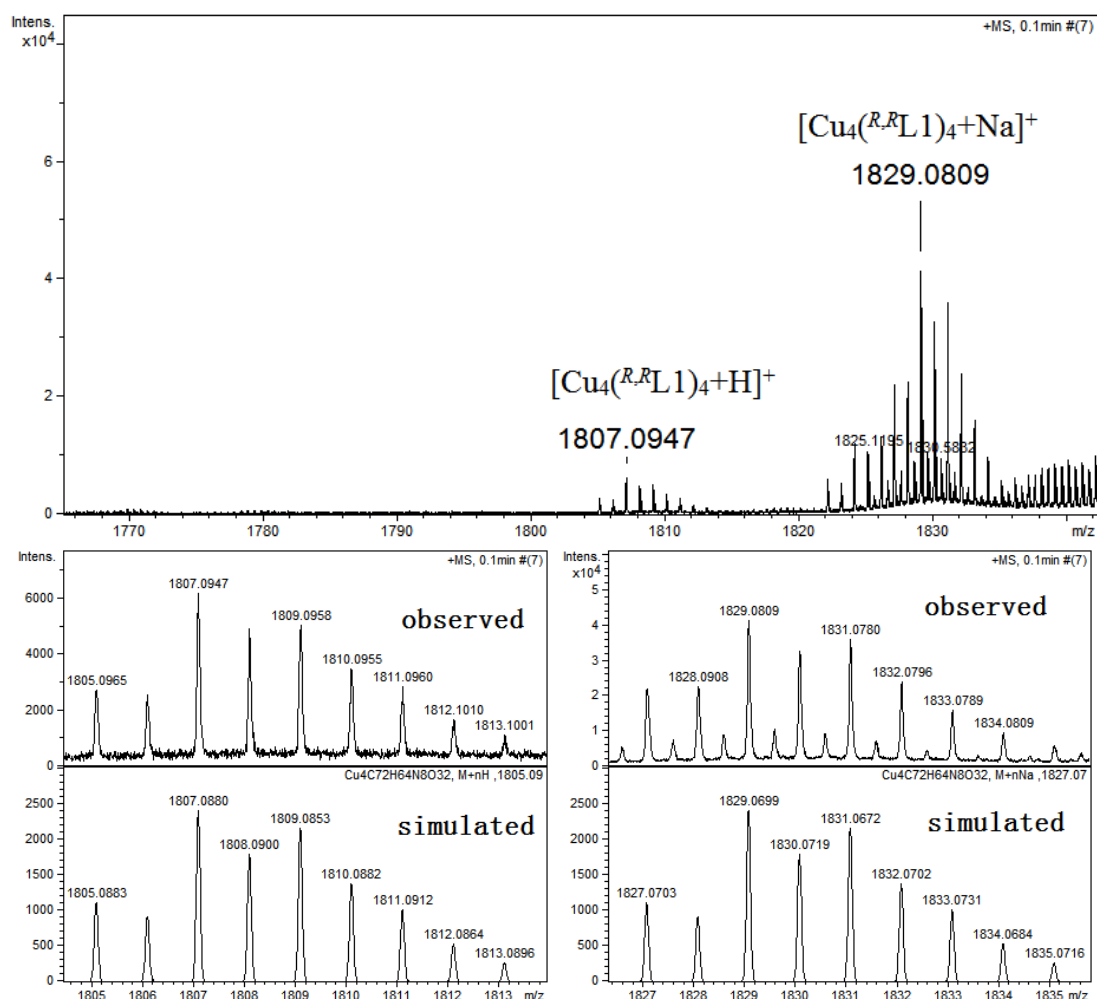


Figure S1b Partial HR-MS(ESI) of **2** in methanol (up). Isotopic distributions and simulations of the $[\text{Cu}_4\text{L}_4+\text{H}]^+$ (down left) and $[\text{Cu}_4\text{L}_4+\text{Na}]^+$ (down right) peaks are amplified.

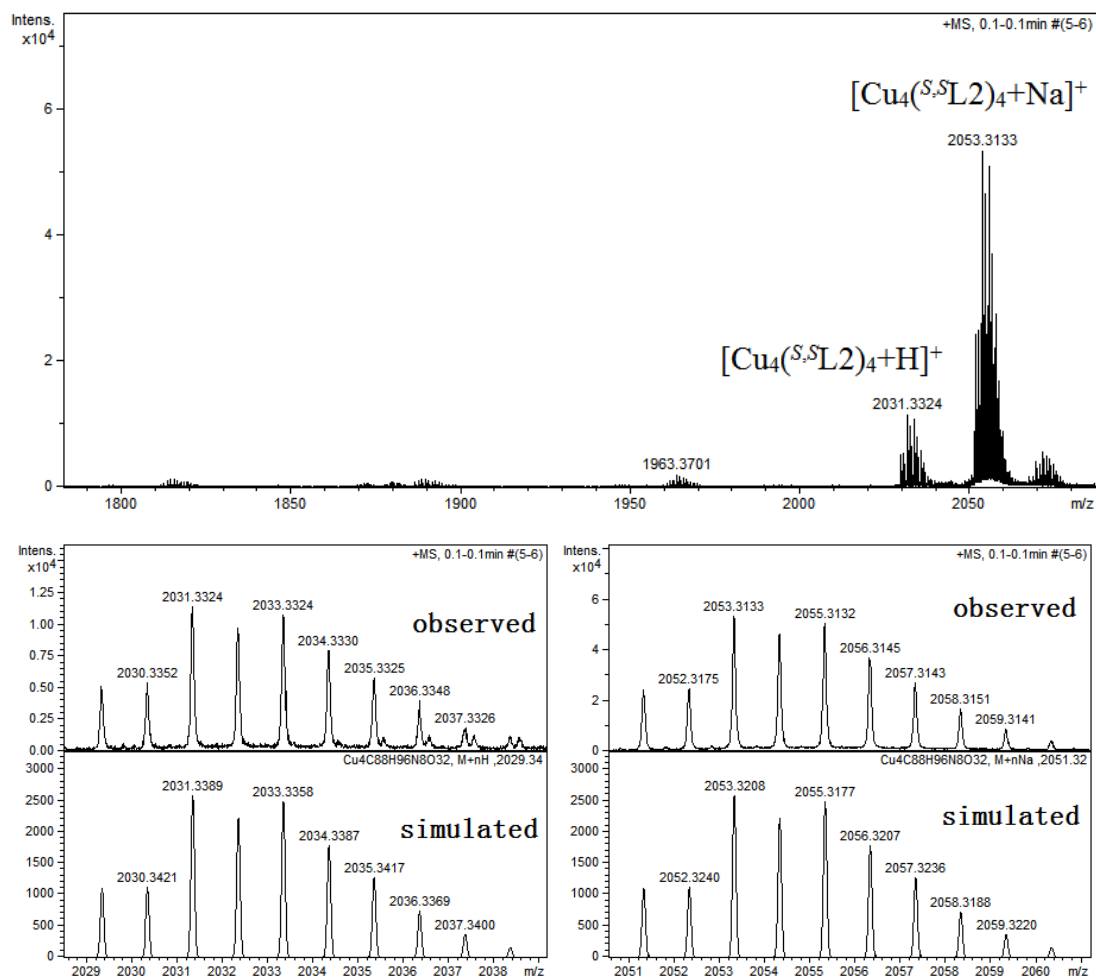


Figure S1c Partial HR-MS(ESI) of **3** in methanol (up). Isotopic distributions and simulations of the $[\text{Cu}_4\text{L}_4+\text{H}]^+$ (down left) and $[\text{Cu}_4\text{L}_4+\text{Na}]^+$ (down right) peaks are amplified.

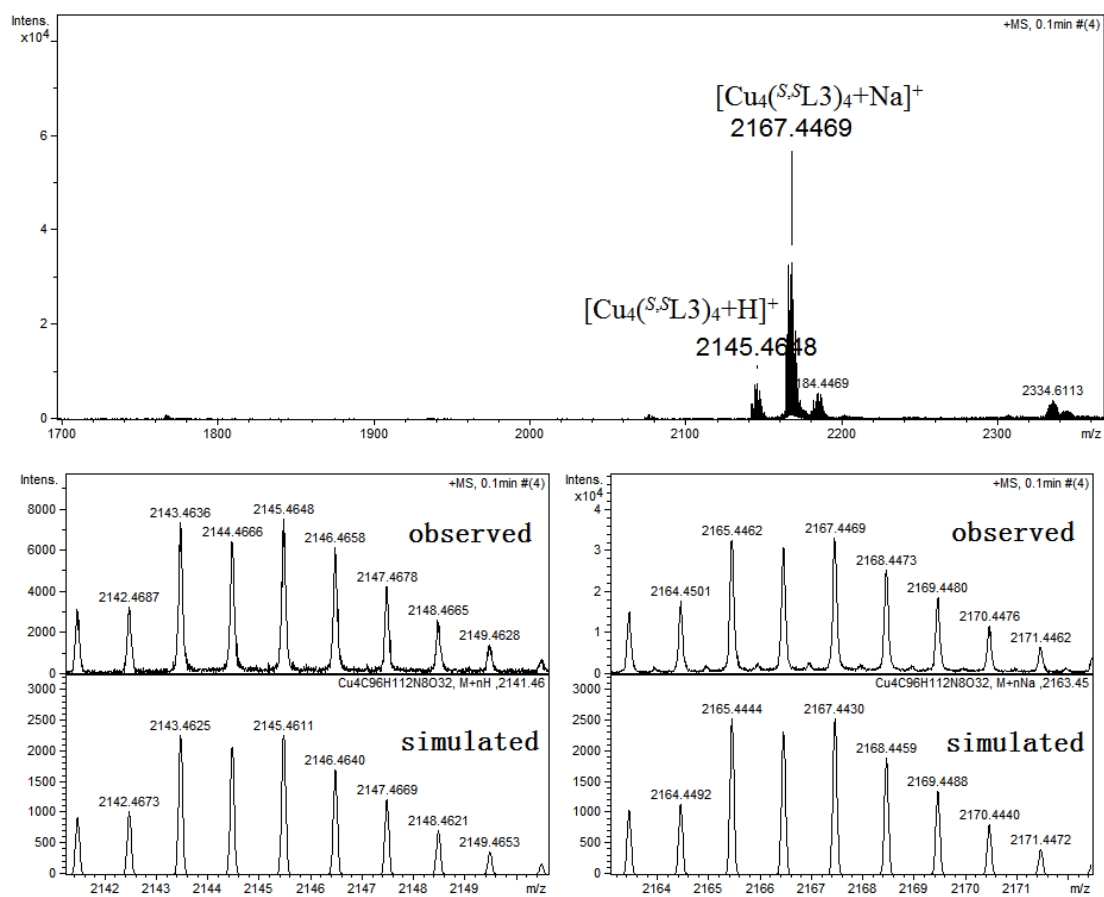


Figure S1d Partial HR-MS(ESI) of **4** in methanol (up). Isotopic distributions and simulations of the $[\text{Cu}_4\text{L}_4+\text{H}]^+$ (down left) and $[\text{Cu}_4\text{L}_4+\text{Na}]^+$ (down right) peaks are amplified.

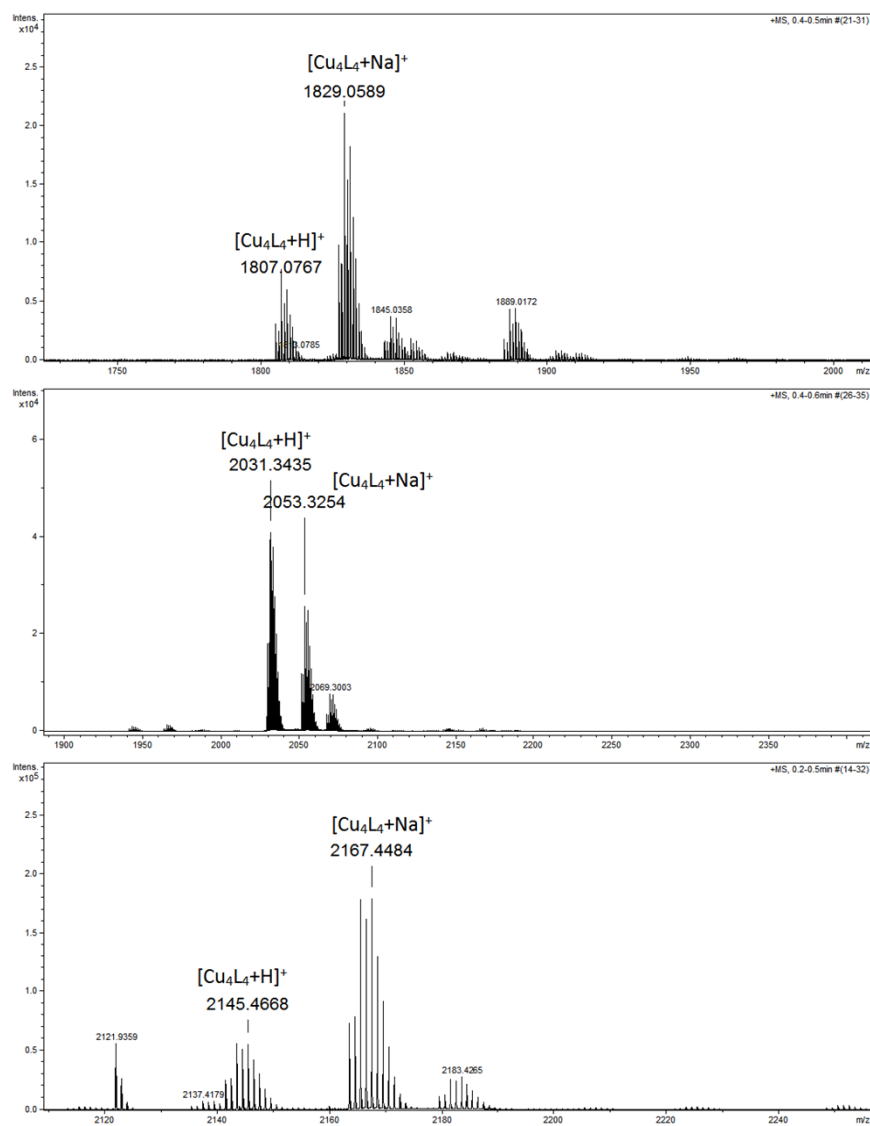


Figure S2 TOF-MS spectra of cage compounds after homogeneous catalytic cyclopropanation reactions in acetone, 1(up); 3(middle); 4(down).

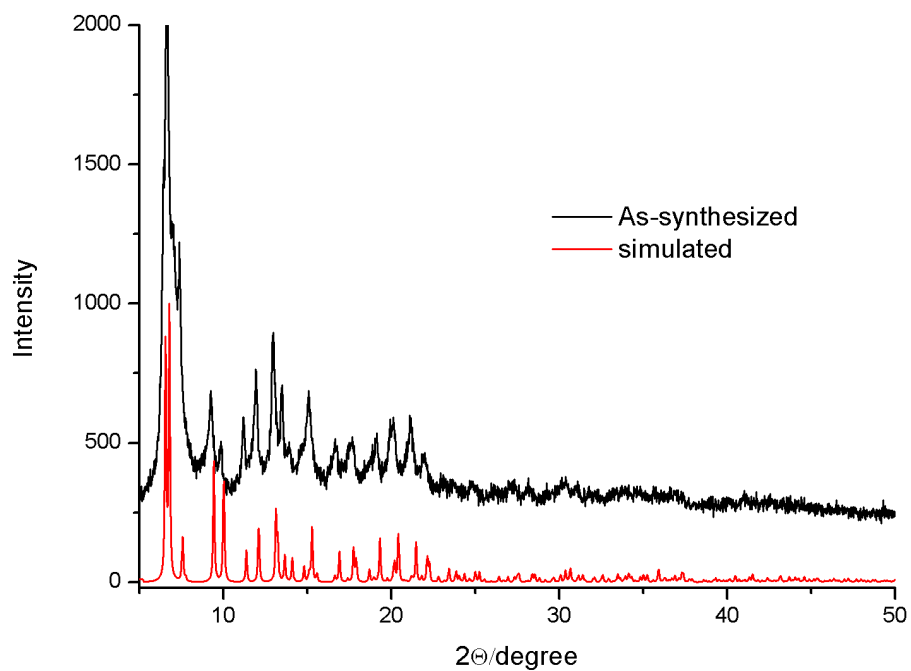


Figure S3a Powder X-ray diffraction (PXRD) patterns of **1**: pattern simulated from single crystal structure in red; observed pattern for the prepared sample in black.

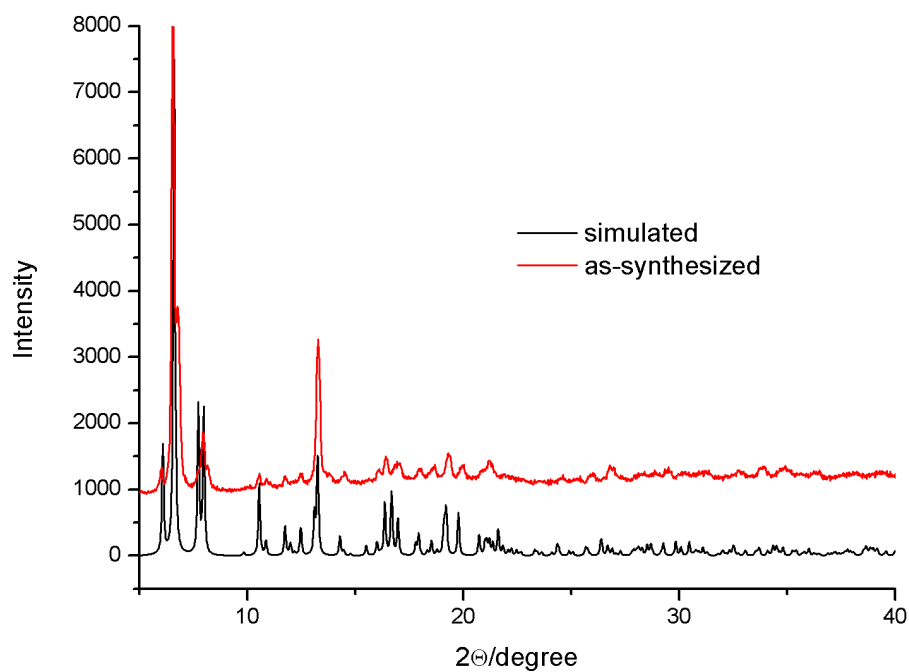


Figure S3b Powder X-ray diffraction (PXRD) patterns of **2**: pattern simulated from single crystal structure in black; observed pattern for the prepared sample in red.

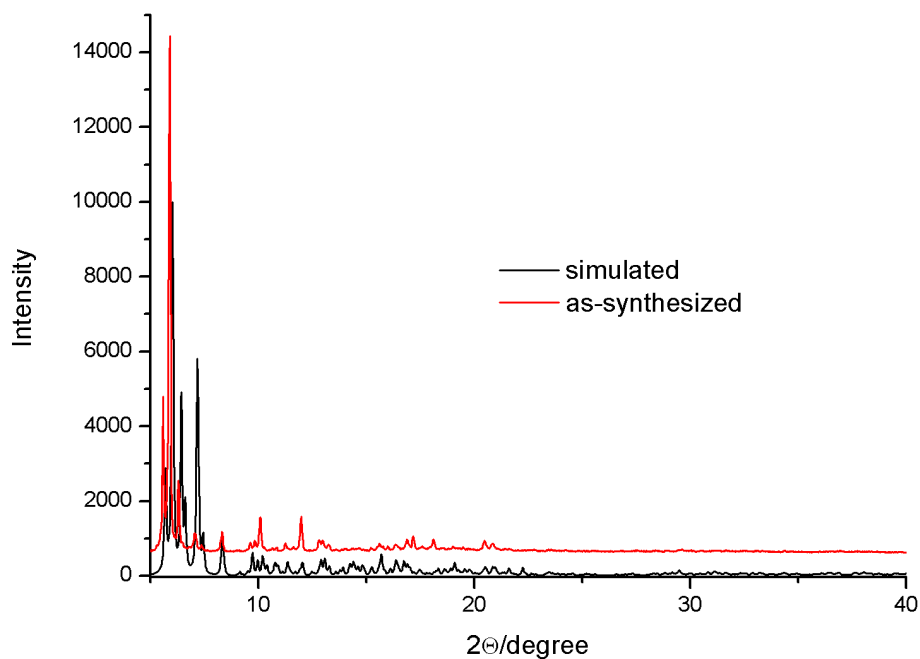


Figure S3c. Powder X-ray diffraction (PXRD) patterns of **3**: pattern simulated from single crystal structure in black; observed pattern for the prepared sample in red.

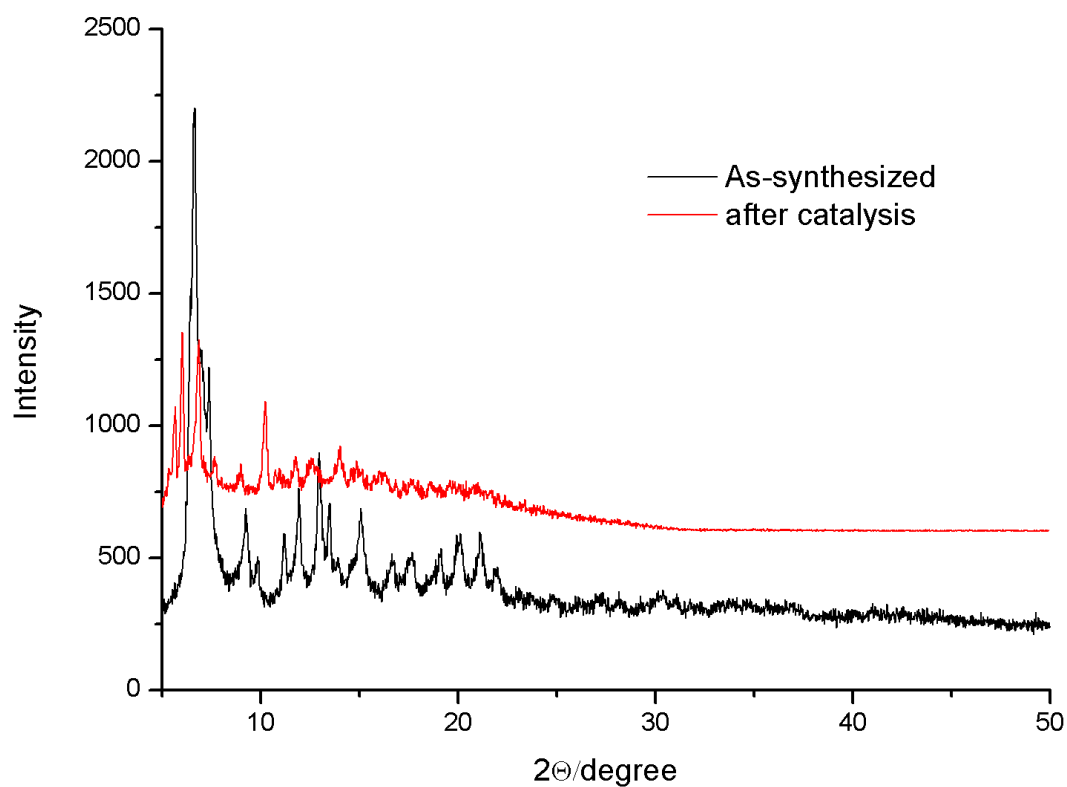


Figure S3d Powder X-ray diffraction (PXRD) patterns of **1**: pattern observed for fresh prepared sample in black; pattern observed for sample after heterogeneous catalytic cyclopropanation in red.

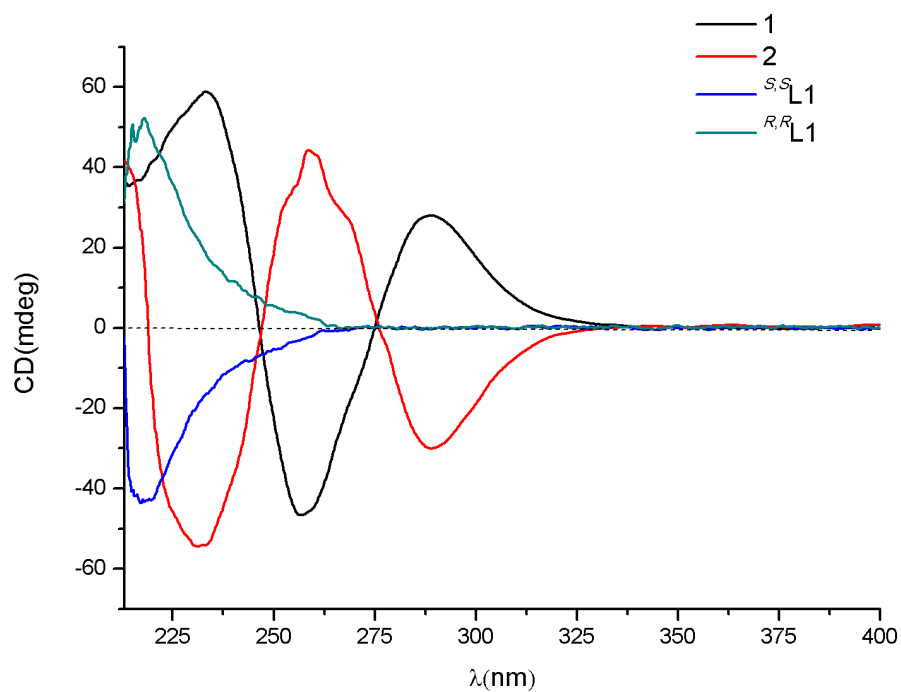


Figure S4 CD spectra of the cage compounds **1**, **2** and ligands S,S -L1, R,R -L1 in methanol.

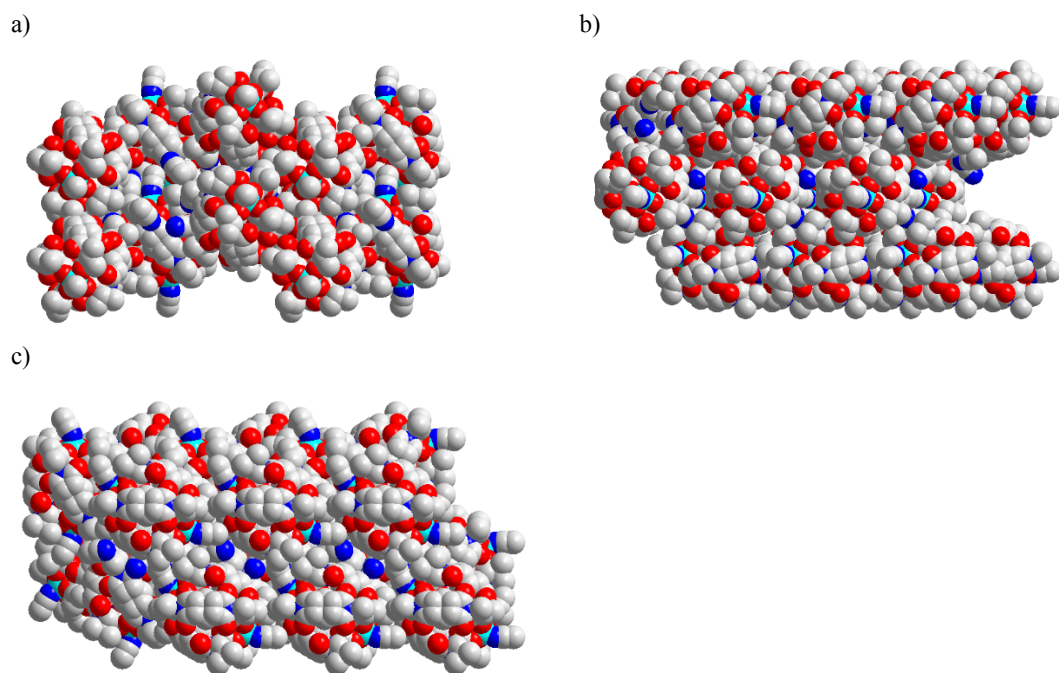


Figure S5 Packing mode of **3** viewed along a, b and c axis for a), b) and c), respectively (space-filling diagram).

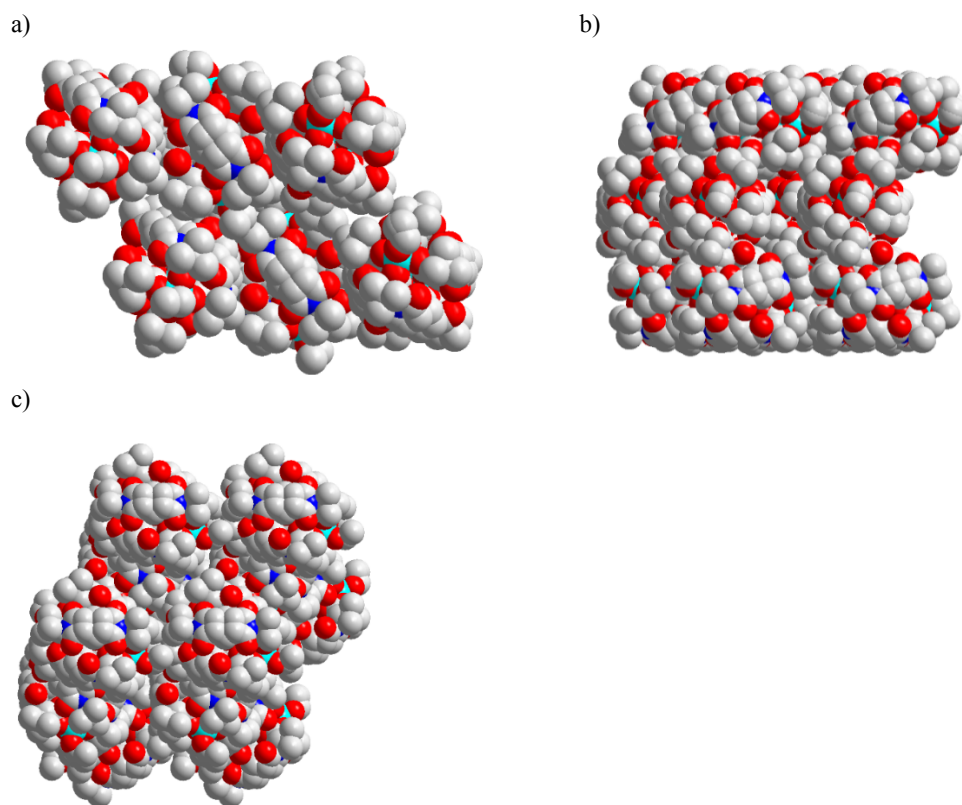


Figure S6 Packing mode of **4** viewed along a, b and c axis for a), b) and c), respectively (space-filling diagram).

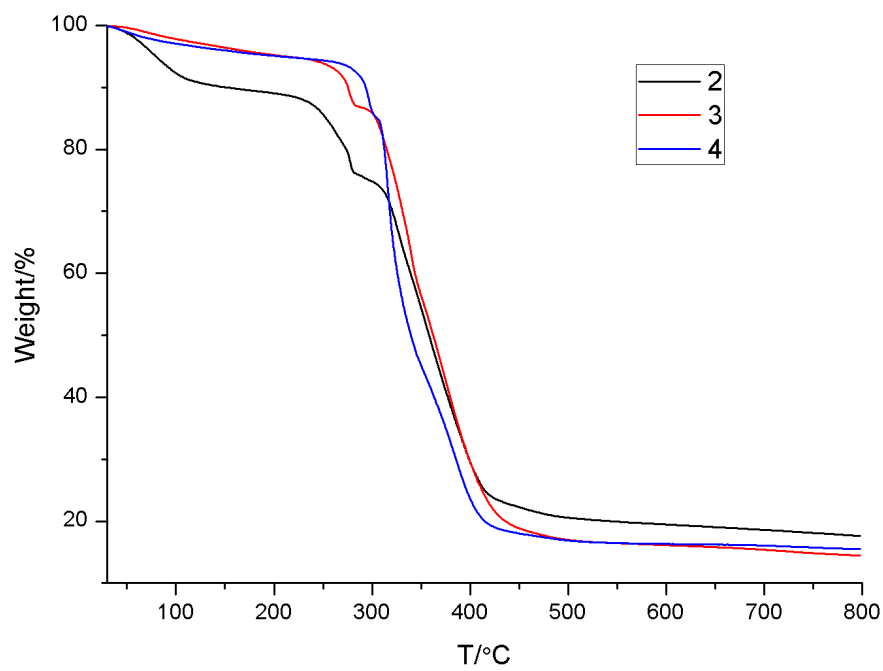


Figure S7 TG curves of **2**, **3** and **4**.