

SUP-DATA

Novel Cu^{II}-M^{II}-Cu^{II} (M = Cu or Ni) trinuclear and [Na^I₂Cu^{II}₆]octanuclear complexes assembled by bi-compartmental ligands: syntheses, structures, magnetic and catalytic studies

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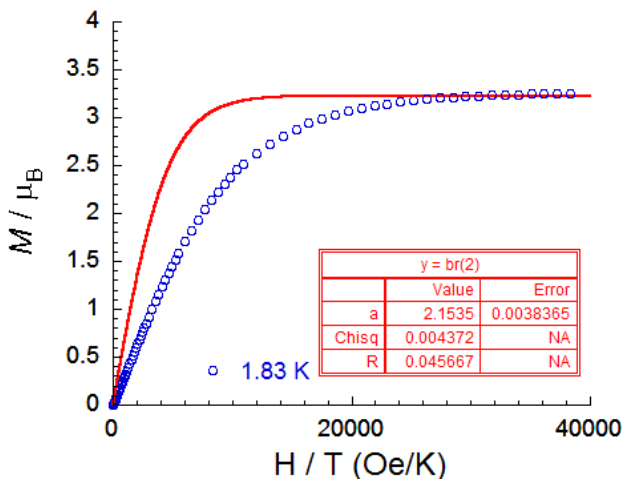


Fig. S1. (left) the M vs H data between 1.83-8 K; (right) the fit of the M vs H/T data at 1.83 K with the $S = 3/2$ Brillouin functions where the blue hollow circle are the experimental data and the solid red line is the fit of the data. This fit displays almost no correspondence to the experimental data (only a few very high field data are correlating the fit).

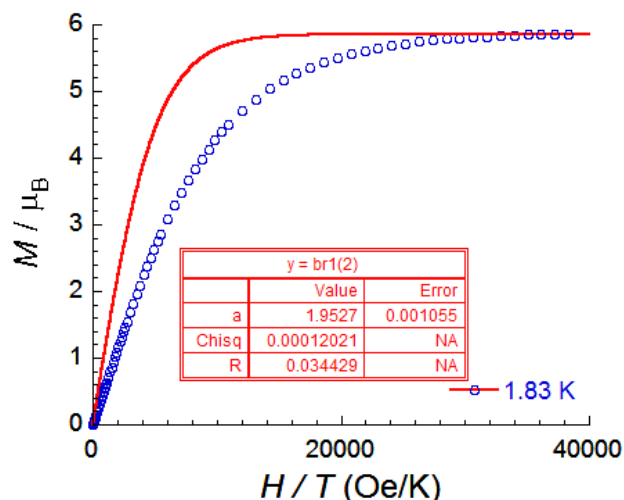


Fig. S2. (left) the M vs H data between 1.83-8 K; (right) the fit of the M vs H/T data at 1.83 K as a pair of the $S=3/2$ Brillouin functions where the blue hollow circle are the experimental data and the solid red line is the fit of the data. This fit displays almost no correspondence to the experimental data (only a few very high field data are correlating the fit).

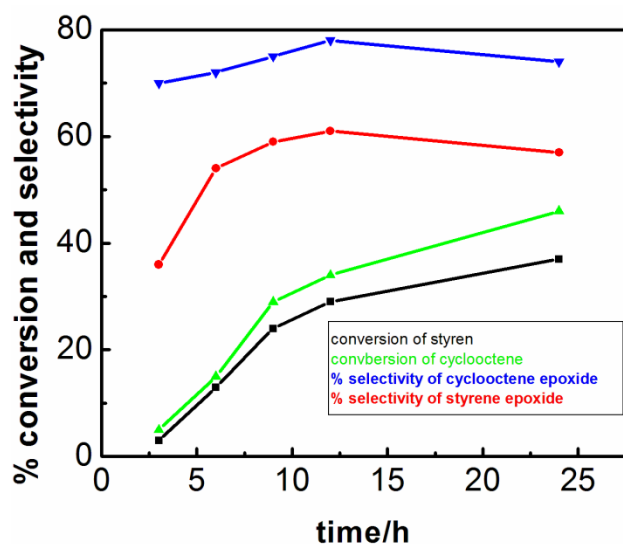


Fig. S3. % Conversions of styrene and cyclooctene at different reaction hours in liquid phase partial oxidation by 5.

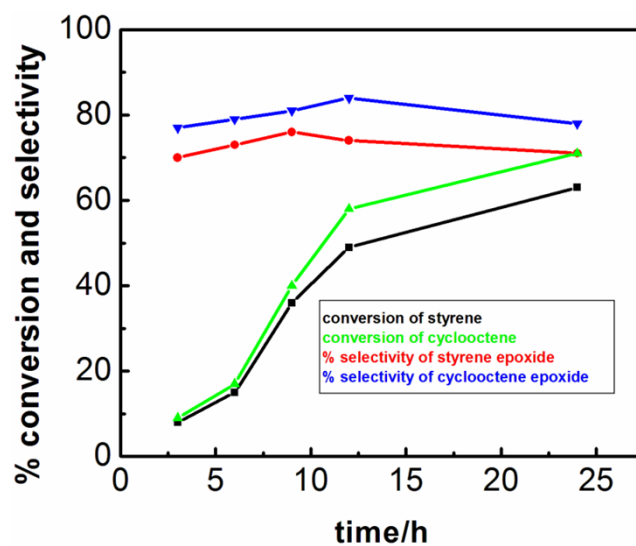
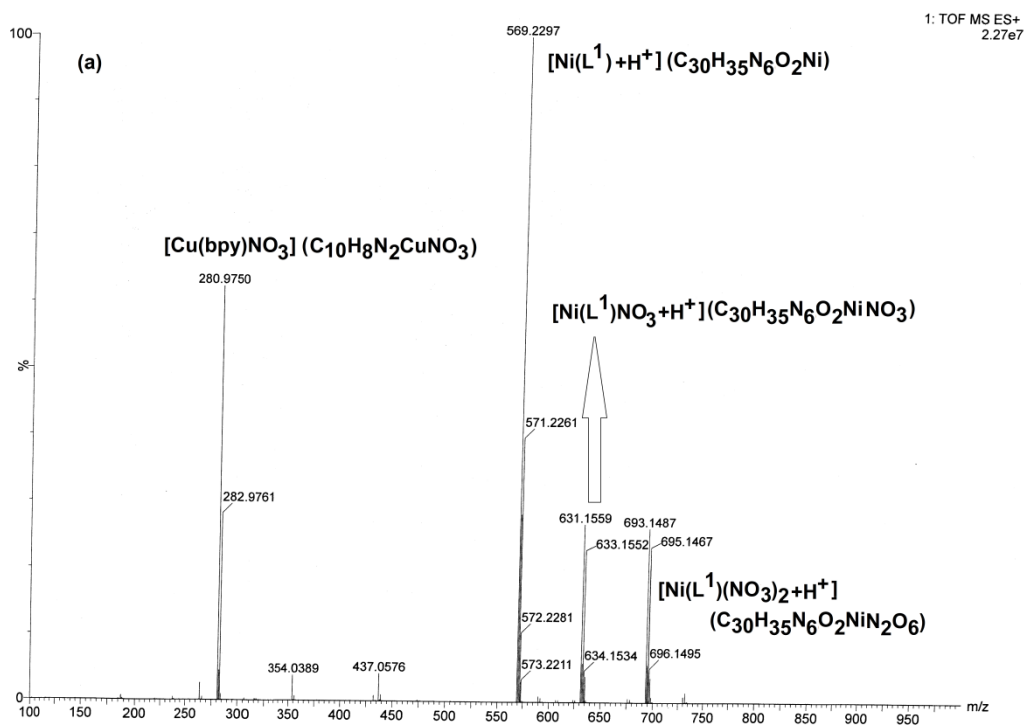
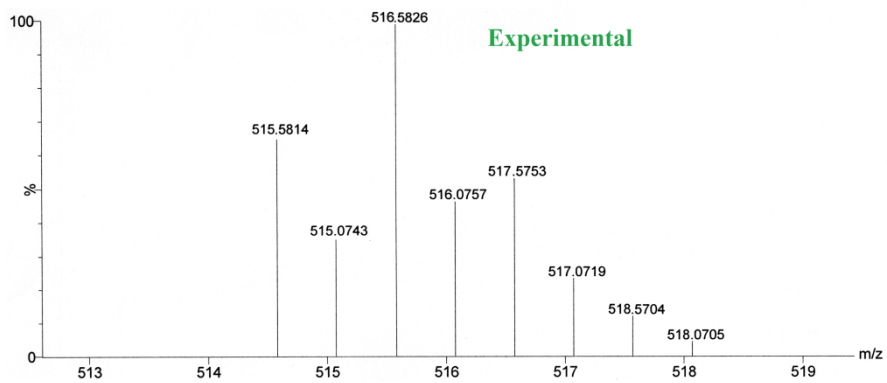
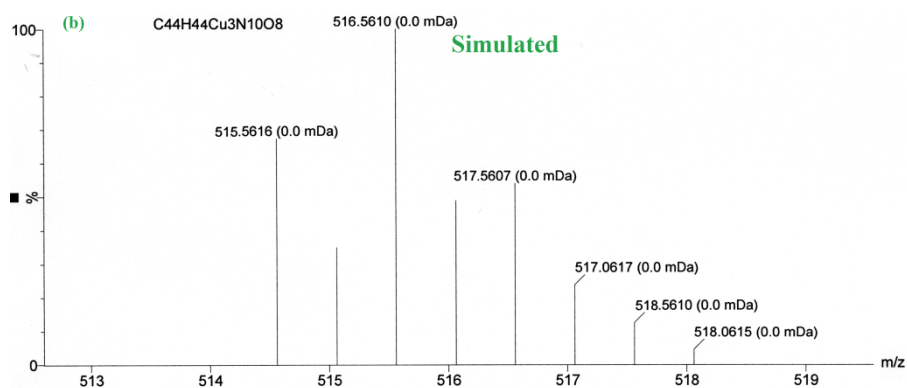
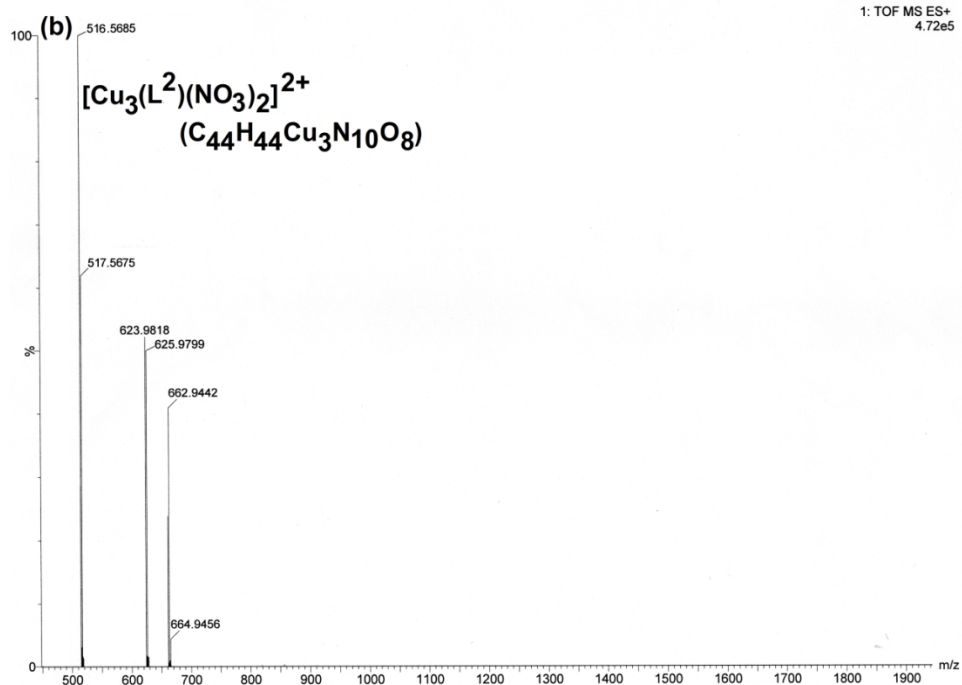


Fig.S4. % Conversions of styrene and cyclooctene at different reaction hours in liquid phase partial oxidation by **6**.





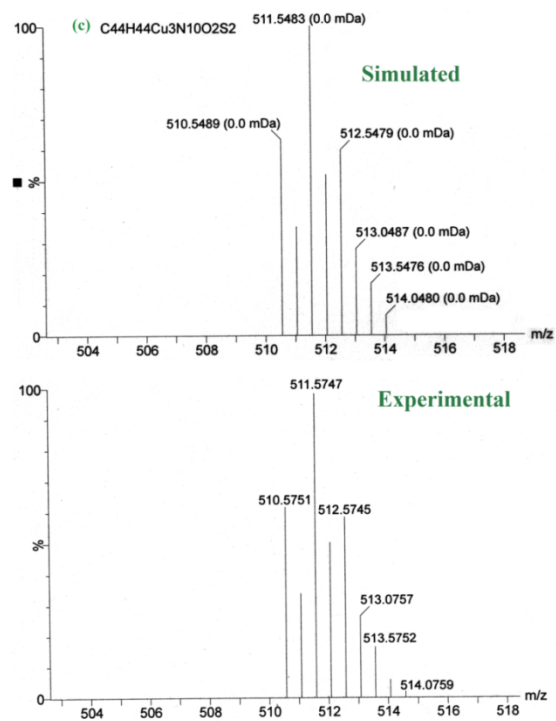
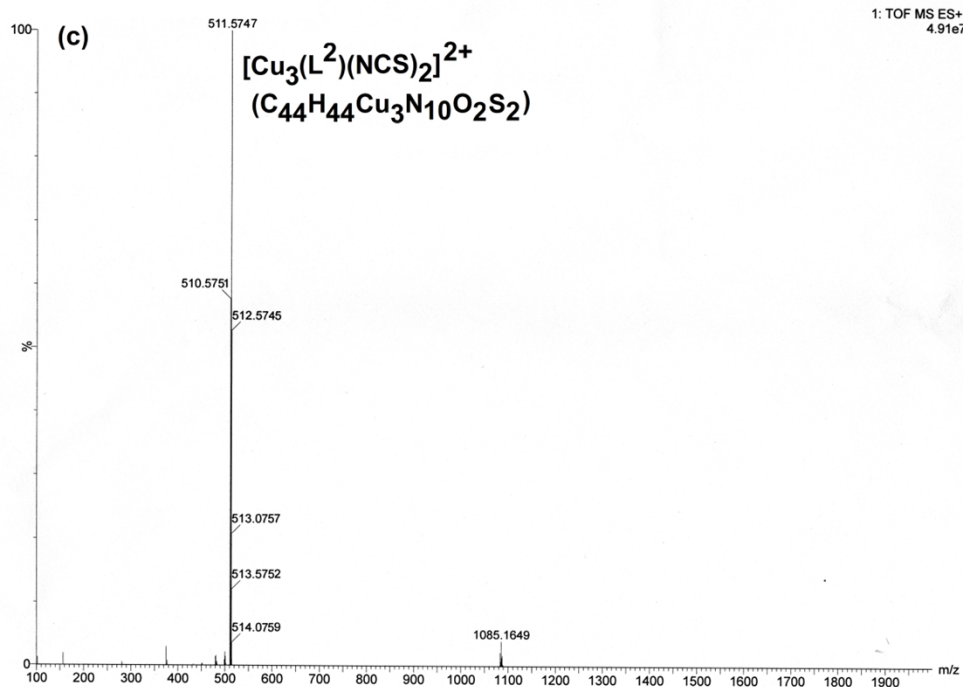


Fig. S5. ES-MS⁺ of (a) complex 5, (b) complex 6 and (c) complex 7.

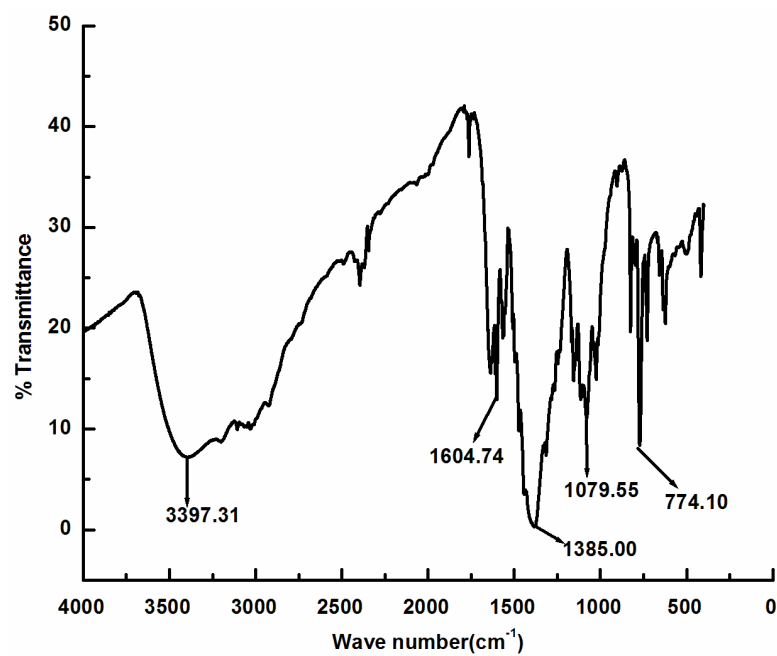


Fig. S6. FTIR of complex 5.

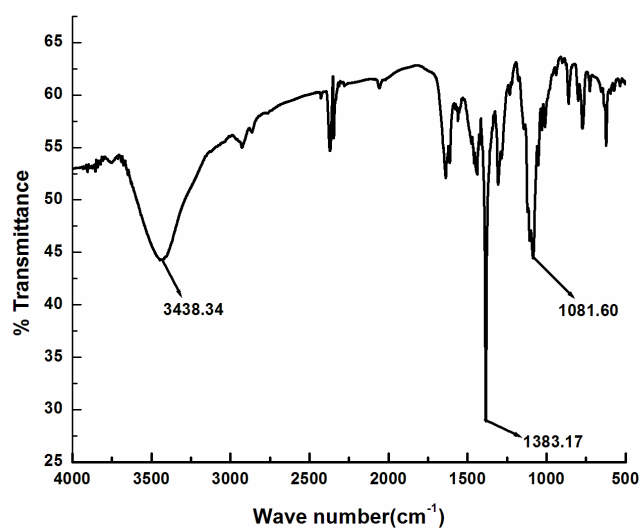


Fig. S7. FTIR of complex 6.

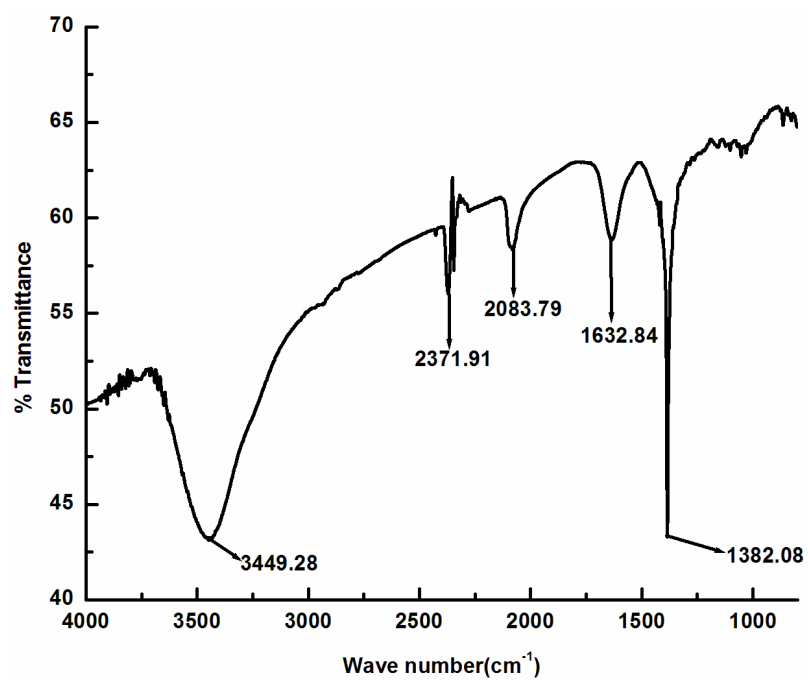


Fig. S8. FTIR of complex 7.

Table S1 Selected Bond lengths (Å) and bond angles (°) of **5**

Bond lengths (Å)		Bond angles (°)	
Cu-O1	1.976(3)	O3-Cu1-N1	130.44(11)
Cu1-O3	2.689(4)	O3-Cu1-N2	85.79(11)
Cu1-O4	2.500(3)	O3-Cu1-N4	79.55(11)
Cu1-N1	2.002(3)	O4-Cu1-N1	83.38(11)
Cu1-N2	2.009(3)	O4-Cu1-N2	107.57(11)
Cu1-N4	1.996(3)	O4-Cu1-N4	94.63(11)
Ni1-O4	1.857(3)	N1-Cu1-N2	80.89(12)
Ni1-N5	1.853(3)	N1-Cu1-N4	94.84(12)
Ni1-O4a	1.857(3)	N2-Cu1-N4	156.61(12)
Ni1-N5a	1.853(3)	O4-Ni1-N5	93.68(13)
Bond Angles(°)		O4-Ni1-O4a	88.11(12)
O1-Cu1-O3	52.60(11)	O4-Ni1-N5a	172.07(13)
O1 -Cu1-O4	94.47(10)	O4a-Ni1-N5	172.07(13)
O1-Cu1-N1	172.94(12)	N5-Ni1-N5a	85.59(14)
O1-Cu1-N2	93.42(12)	O4a-Ni1-N5a	93.68(13)
O1-Cu1-N4	92.03(12)	Cu1-O1-N6	110.6(3)
O3-Cu1-O4	145.82(10)	Cu1-O3-N6	78.0(2)
		Cu1-O4-Ni1	103.40(11)
		Cu1-N4-N3	127.3(2)

Symmetry operators: x,y,z; 1/2-x,y,1/2-z; -x,-y,-z; 1/2+x,-y,1/2+z.

Table S2 Selected Bond lengths (Å) and bond angles (°) of **6**

Bond lengths (Å)			
Cu1-O1	1.961(4)	O4 -Cu1 -O4a	147.36(16)
Cu1-O4	2.600(5)	O4 -Cu1 -N1a	98.71(17)
Cu1-N1	1.927(5)	O1a -Cu1 -N1	167.53(19)
Cu1-O1a	1.961(4)	Cu1 -O1 -Cu2	108.6(2)
Cu1-O4a	2.600(5)	O4a -Cu1 -N1	98.71(17)
Cu1-N1a	1.927(5)	N1 -Cu1 -N1a	82.8(2)
Cu2 -O1	2.285(5)	O1a -Cu1 -O4a	73.32(17)
Cu2 -O3	2.776(7)	Cu1 -O4 -Cu2	97.19(18)
Cu2 -O4	1.970(5)	O1a -Cu1 -N1a	90.07(19)
Cu2 -N2	2.025(7)	O4a -Cu1 -N1a	105.67(17)
Cu2 -N3	1.919(7)	O1 -Cu2 -O3	130.61(18)
Cu2 -N4	1.975(7)	O1 -Cu2 -O4	80.90(17)
Bond angles (°)		O1 -Cu2 -N2	93.2(2)
		O1 -Cu2 -N3	91.3(2)
O1 -Cu1 -O4	73.32(17)	O1 -Cu2 -N4	100.17(17)
O1 -Cu1 -N1	90.07(19)	O3 -Cu2 -O4	49.7(2)
O -Cu1 -O1a	98.66(17)	O3 -Cu2 -N2	136.2(2)
O1 -Cu1 -O4a	85.46(17)	O3 -Cu2 -N3	94.4(2)
O1 -Cu1 -N1a	167.5(2)	O3 -Cu2 -N4	87.9(2)
O4 -Cu1 -N1	105.67(17)	O4 -Cu2 -N2	173.7(2)
O1a -Cu1 -O4	85.46(17)	O4 -Cu2 -N3	98.5(3)
		O4 -Cu2 -N4	96.1(3)
		N2 -Cu2 -N3	83.6(3)

Symmetry operators: a= -x,y,1/2-z