Supporting Information

Formation of N-oxido copper ethylenediaminetetraacetate and propanediaminetetraacetate and their selective degradations to iminodiacetate and propanediaminediacetate

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Figure S1

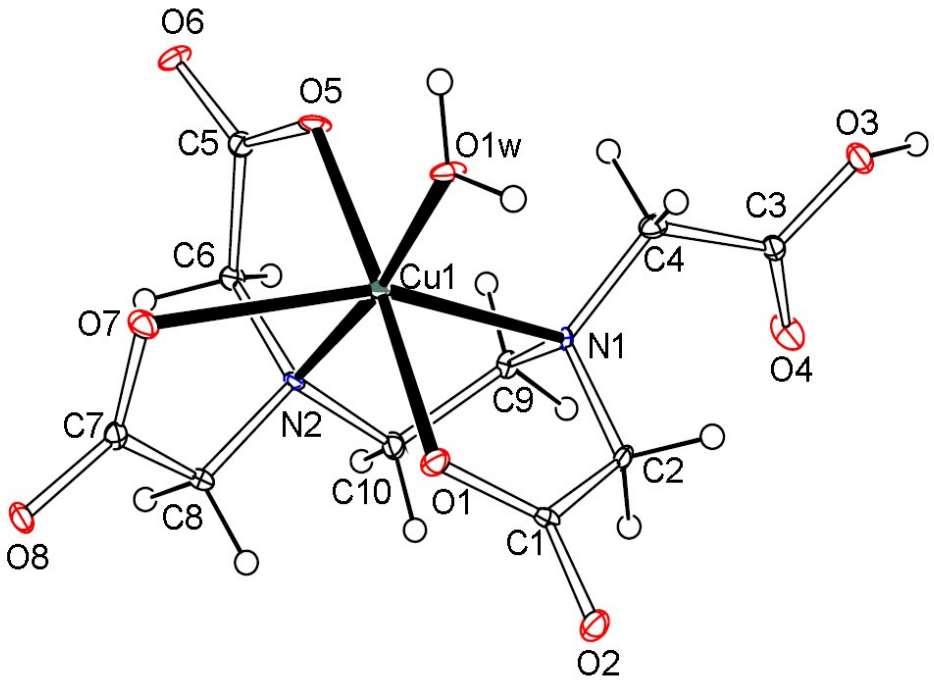

Figure S2

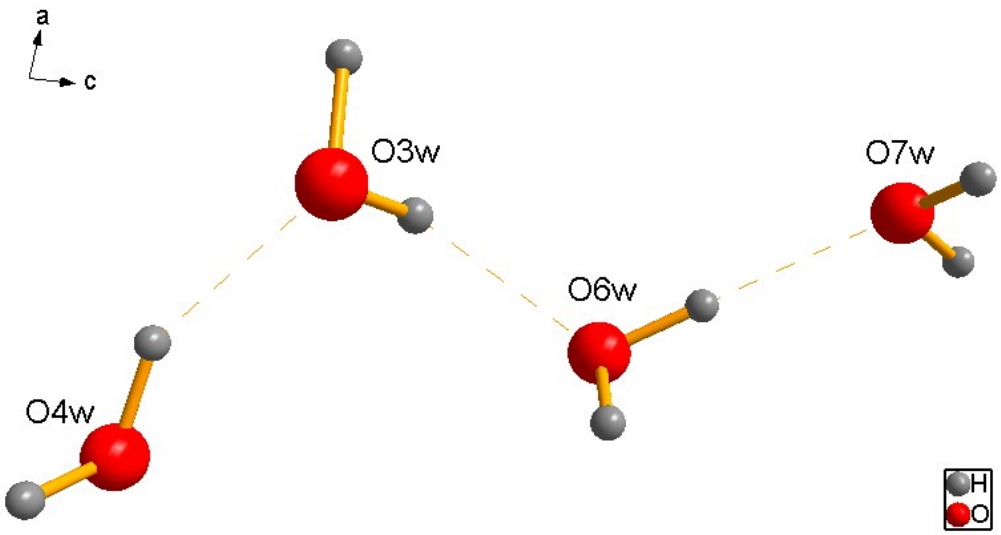

Figure S3

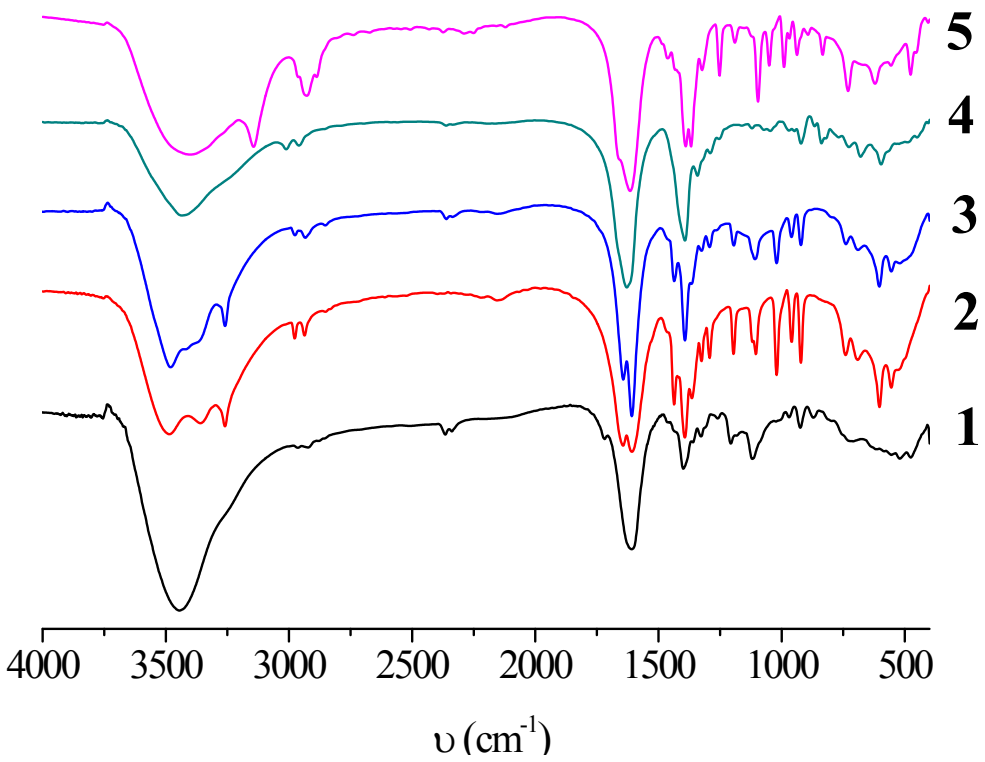

Table S1. Selected bond distances for K[Cu(Hedta)(H_2O)] (**1**), $Na_{4n}[Cu_2(edtaO_2)_2(H_2O)_4]_n \cdot 13nH_2O$ (**2**), K[Cu(ida)(H_2O)$_2$Cl] (**3**), $Na_{5n}O_n[Cu_2(HpdtaO_2)_2Cl]_n \cdot 12.5nH_2O$ (**4**) and $[Cu_2(pdda)_2]_n \cdot nH_2O$ (**5**).

Bonds	**1**	Bonds	**2**	Bonds	**3**	Bonds	**4**	Bonds	**5**
Cu(1)–O(1)	1.967(4)	Cu(1)–O(1)	1.954(3)	Cu(1)–O(1)	1.969(3)	Cu(1)–O(1)	1.957(5)	Cu(1)–O(1)	1.948(2)
Cu(1)–O(5)	1.939(4)	Cu(1)–O(1a)	1.954(3)	Cu(1)–O(3)	1.969(3)	Cu(1)–O(2a)	2.988(5)	Cu(1)–O(3)	1.982(2)
Cu(1)–O(7)	2.488(4)	Cu(1)–O(9)	1.926(3)	Cu(1)–O(1w)	2.556(3)	Cu(1)–O(9)	1.938(5)	Cu(1)–O(2a)	2.221(2)
Cu(1)–O(1w)	1.968(4)	Cu(1)–O(9a)	1.926(3)	Cu(1)–O(2w)	2.413(3)	Cu(1)–O(11)	1.958(5)	Cu(1)–N(1)	2.001(2)
Cu(1)–N(1)	2.340(4)	Cu(1)–O(5w)	2.645(3)	Cu(1)–N(1)	1.999(4)	Cu(1)–O(19)	1.917(5)	Cu(1)–N(2)	2.001(2)
Cu(1)–N(2)	2.054(5)	Cu(1)–O(5wa)	2.645(3)	Cu(1)–Cl(1)	2.281(1)	Cu(2)–O(5)	1.960(5)	Cu(1)–O(1w)	3.611(2)
		Cu(2)–O(7)	1.965(3)			Cu(2)–O(10)	1.918(5)		
		Cu(2)–O(7b)	1.965(3)			Cu(2)–O(15)	1.947(5)		
		Cu(2)–O(10)	1.934(3)			Cu(2)–O(16b)	3.131(6)		
		Cu(2)–O(10b)	1.934(3)			Cu(2)–O(20)	1.929(5)		
		Cu(2)–O(8w)	2.481(3)			Cu(1)–Cl(1)	2.757(2)		
		Cu(2)–O(8wb)	2.481(3)			Cu(2)–Cl(1)	2.756(2)		

Symmetry transformations: for **2**, (a) $-x + 1, -y + 2, -z$; (b) $-x + 1, -y + 1, -z + 1$; for **4**, (a) $-x + 1, -y + 2, -z + 1$; (b) $-x + 2, -y + 1, -z$; for **5**, (a) $-x + ½, y + ½, -z + ½$.

Table S2. Selected bond distances and angles within the water clusters in $Na_{4n}[Cu_2(edtaO_2)_2(H_2O)_4]_n \cdot 13nH_2O$ (**2**).

D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A(°)
O3w–H…O6wa	0.81(9)	2.09(8)	2.873(7)	161(7)
O4w–H…O3wb	0.92(8)	1.99(8)	2.789(8)	144(8)
O6w–H…O7wc	0.91(7)	1.85(7)	2.745(7)	168(7)

Symmetry transformations: (a) -*x* + 1, -*y* + 2, -*z*; (b) -*x* + 1, -*y* + 2, -*z* + 1; (c) -*x* + 1, -*y* + 1, -*z*.

Table S3. Bond valence sum calculations for copper complexes **1** ~ **5**.

Cu^{2+}	Complexes	Cu1	Cu2
+2	K[Cu(Hedta)(H_2O)] (**1**)	1.965	
+2	$Na_{4n}[Cu_2(edtaO_2)_2(H_2O)_4]_n \cdot 13nH_2O$ (**2**)	2.124	2.156
+2	$K[Cu(ida)(H_2O)_2Cl]$ (**3**)	1.806	
+2	$Na_{5n}[Cu_2(pdtaO_2)_2Cl]_n \cdot 12.5nH_2O$ (**4**)	2.080	2.092
+2	$[Cu_2(pdda)_2]_n \cdot nH_2O$ (**5**)	1.856	