Supporting Information

Mono- or multinuclear Copper(II), Nickel(II) and Cobalt(III) Complexes with in Situ Schiff Base Ligands from a Linear Polyamine : Synthesis, Structures and Magnetic Properties

Caixia Ding, Jia Ni, Yuhua Yang, Seik Weng Ng, Bingwu Wang*, Yongshu Xie*

Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science & Technology, Shanghai 200237, P. R. China. Department of Chemistry, Shantou University, Shantou, 515063, P. R. China. Department of Chemistry, University of Malaya, 50603, Kuala Lumpur, Malaysia. Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia. Beijing National Laboratory of Molecular Science, State Key Laboratory of Rare Earth Materials Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, P. R. China.

Corresponding Author: *Yongshu Xie
Telephone number: (86)-21-64250772
E-mail address: yshxie@ecust.edu.cn

Table S1. Selected Bond Lengths (Å) and Angles (˚) for the Metal Complexes **1** ~ **4**.

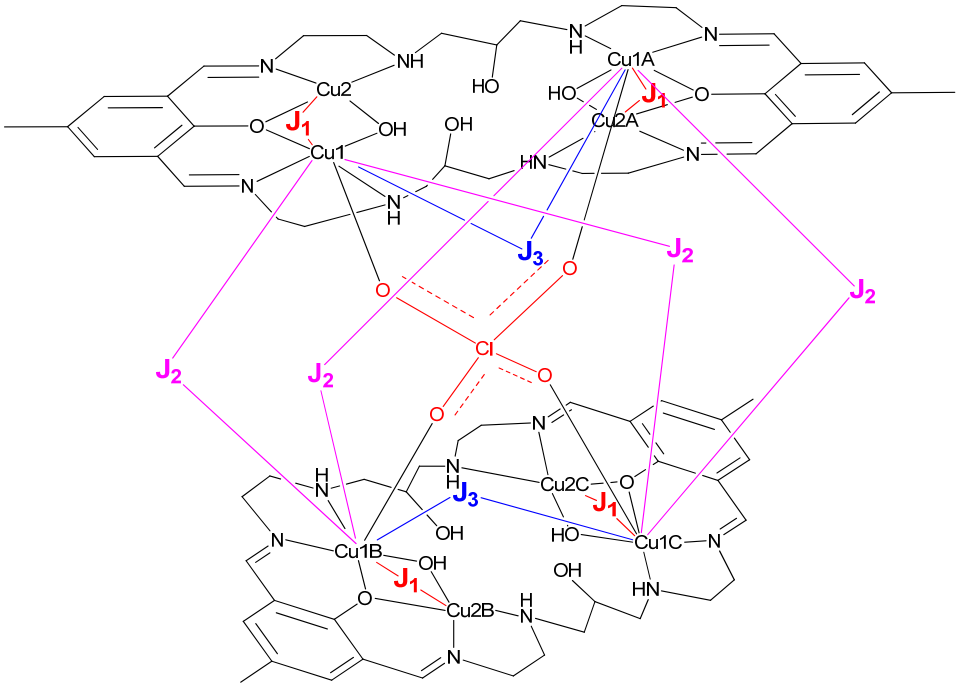
Complex **1**

Co(1)-O(2)#1	1.892(2)	O(2)#1-Co(1)-O(2)	89.87(16)	O(2)#1-Co(1)-N(2)#1	177.50(12)	O(2)-Co(1)-N(2)	177.50(12)
Co(1)-O(2)	1.892(2)	O(2)#1-Co(1)-N(1)	86.11(12)	O(2)-Co(1)-N(2)#1	88.76(12)	N(1)-Co(1)-N(2)	84.94(14)
Co(1)-N(1)	1.900(3)	O(2)-Co(1)-N(1)	92 .89(12)	N(1)-Co(1)-N(2)#1	96.04(14)	N(1)#1-Co(1)-N(2)	96.04(14)
Co(1)-N(1)#1	1.900(3)	O(2)#1-Co(1)-N(1)#1	92.89(12)	N(1)#1-Co(1)-N(2)#1	84.94(14)	N(2)#1-Co(1)-N(2)	92.68(18)
Co(1)-N(2)#1	1.960(3)	O(2)-Co(1)-N(1)#1	86.11(12)	O(2)#1-Co(1)-N(2)	88.76(12)	N(1)-Co(1)-N(1)#1	178.60(19)
Co(1)-N(2)	1.960(3)						

Symmetry transformations used to generate equivalent atoms: #1 -x+1, y, -z+1/2

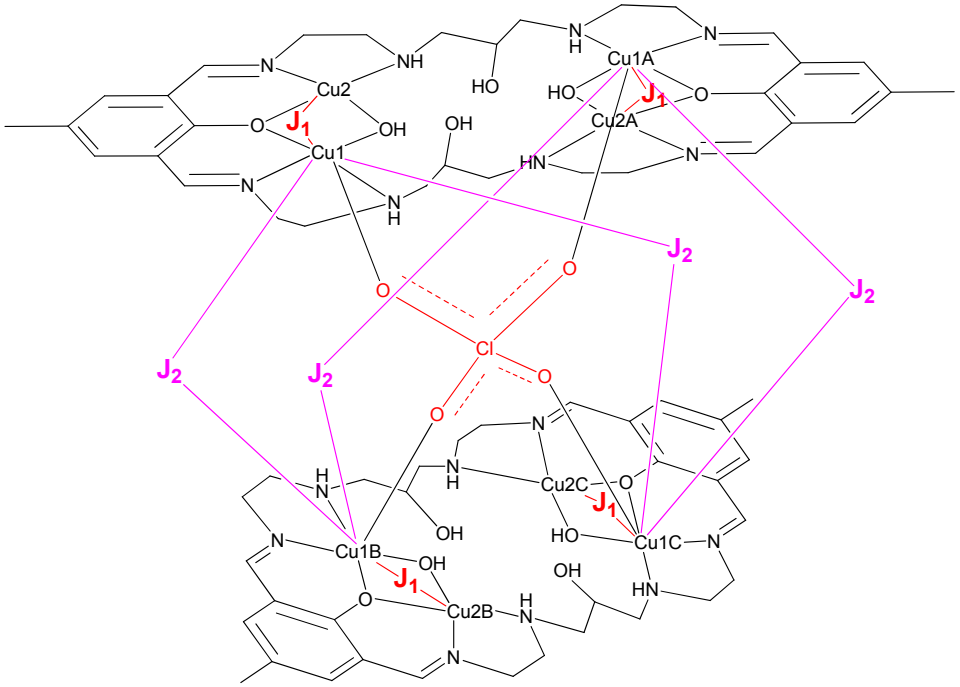
Complex **2**							
Ni(1)-O(2)	1.844(3)	Ni(1)-N(2)	1.920(4)	O(2)-Ni(1)-N(1)	94.06(14)	O(2)-Ni(1)-N(3)	84.71(13)
Ni(1)-N(1)	1.858(4)	N(1)-Ni(1)-N(2)	86.41(16)	O(2)-Ni(1)-N(2)	178.40(16)	N(1)-Ni(1)-N(3)	177.93(15)
Ni(1)-N(3)	1.957(3)	N(2)-Ni(1)-N(3)	94.87(15)				
Complex **3**							
Ni(1)-N(8)	2.005(9)	N(8)-Ni(1)-N(9)	94.8(4)	N(7)-Ni(1)-O(5)	94.1(3)	Ni(4)-N(6)	1.869(8)
Ni(1)-N(9)	2.036(10)	N(8)-Ni(1)-O(1)	87.1(3)	N(4)-Ni(2)-N(11)	91.4(4)	O(1)-Ni(3)-N(1)	96.8(4)
Ni(1)-O(1)	2.061(7)	N(9)-Ni(1)-O(1)	91.8(3)	N(4)-Ni(2)-O(4)	162.3(3)	O(1)-Ni(3)-O(2)	85.4(3)
Ni(1)-O(2)	2.068(7)	N(8)-Ni(1)-O(2)	160.5(3)	N(11)-Ni(2)-O(4)	90.8(3)	N(1)-Ni(3)-O(2)	175.5(3)
Ni(1)-N(7)	2.122(8)	N(9)-Ni(1)-O(2)	91.8(3)	N(4)-Ni(2)-O(3)	87.0(3)	O(1)-Ni(3)-N(2)	174.2(3)
Ni(1)-O(5)	2.127(8)	O(1)-Ni(1)-O(2)	74.4(3)	N(11)-Ni(2)-O(3)	92.0(3)	N(1)-Ni(3)-N(2)	88.7(4)
Ni(2)-N(4)	2.014(9)	N(8)-Ni(1)-N(7)	84.6(4)	O(4)-Ni(2)-O(3)	75.3(3)	O(2)-Ni(3)-N(2)	89.0(3)
Ni(2)-N(11)	2.056(10)	N(9)-Ni(1)-N(7)	87.2(3)	N(4)-Ni(2)-N(3)	84.4(4)	N(5)-Ni(4)-O(3)	95.9(4)
Ni(2)-O(4)	2.056(7)	O(1)-Ni(1)-N(7)	171.6(3)	N(11)-Ni(2)-N(3)	93.1(3)	N(5)-Ni(4)-O(4)	176.3(4)
Ni(2)-O(3)	2.076(7)	O(2)-Ni(1)-N(7)	114.0(3)	O(4)-Ni(2)-N(3)	113.0(3)	O(3)-Ni(4)-O(4)	86.4(3)
Ni(2)-N(3)	2.101(8)	N(8)-Ni(1)-O(5)	91.1(3)	O(3)-Ni(2)-N(3)	170.1(3)	N(5)-Ni(4)-N(6)	88.4(4)
Ni(2)-N(10)	2.175(10)	N(9)-Ni(1)-O(5)	174.1(3)	N(4)-Ni(2)-N(10)	89.4(4)	O(3)-Ni(4)-N(6)	175.0(3)
Ni(3)-O(1)	1.836(7)	O(1)-Ni(1)-O(5)	87.7(3)	O(4)-Ni(2)-N(10)	88.5(3)	O(4)-Ni(4)-N(6)	89.1(3)
Ni(3)-N(1)	1.839(9)	O(2)-Ni(1)-O(5)	82.4(3)	O(3)-Ni(2)-N(10)	88.5(3)	Ni(3)-O(2)-Ni(1)	99.8(3)
Ni(3)-O(2)	1.844(7)	N(11)-Ni(2)-N(10)	179.0(4)	N(3)-Ni(2)-N(10)	86.5(3)	Ni(4)-O(3)-Ni(2)	98.5(3)
Ni(4)-N(5)	1.820(9)	Ni(3)-N(2)	1.876(9)	Ni(3)-O(1)-Ni(1)	100.3(3)	Ni(4)-O(4)-Ni(2)	99.2(3)
Ni(4)-O(4)	1.846(7)	Ni(4)-O(3)	1.843(7)				
Complex **4**							
Cu(1)-O(5)	1.877(5)	Cu(2)-O(5)	1.896(5)	O(5)-Cu(1)-N(1)	165.0(2)	N(1)-Cu(1)-N(2)	84.5(2)
Cu(1)-N(1)	1.937(5)	Cu(2)-O(1)	1.952(4)	O(5)-Cu(1)-O(1)	78.1(2)	O(1)-Cu(1)-N(2)	172.3(2)
Cu(1)-O(1)	1.983(4)	N(4)#1-Cu(2)-O(1)	92.0(2)	N(1)-Cu(1)-O(1)	90.2(2)	O(5)-Cu(1)-O(3)	89.3(2)
Cu(1)-N(2)	2.038(6)	O(5)-Cu(2)-O(1)	78.4(2)	O(5)-Cu(1)-N(2)	106.2(2)	N(1)-Cu(1)-O(3)	100.4(2)
Cu(1)-O(3)	2.389(5)	N(4)#1-Cu(2)-N(3)#1	86.1(3)	Cu(2)-O(1)-Cu(1)	98.4(2)	O(1)-Cu(1)-O(3)	90.68(18)
N(3)-Cu(2)#1	1.997(6)	O(5)-Cu(2)-N(3)#1	103.8(3)	Cu(1)-O(5)-Cu(2)	104.2(2)	N(2)-Cu(1)-O(3)	95.7(2)
N(4)-Cu(2)#1	1.887(7)			O(1)-Cu(2)-N(3)#1	175.6(3)	N(4)#1-Cu(2)-O(5)	169.1(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y+3/2, z



3-J Model

Scheme S1. Magnetic exchange pathways for complex **4** assuming three different J values.



2-J Model

Scheme S2. Magnetic exchange pathways for complex **4** assuming two different J values.