

Keggin POM-based 3D Framework Tuned by Silver Polymeric Motifs: Structural Influences of Tetrazolate Functional Groups

Xiang Wang^{a, b}, Jun Peng^{a*}, Kundawlet Alimaje^a, Zhenyu Shi^a

^a Key Laboratory of Polyoxometalate Science of Ministry of Education, Faculty of Chemistry, Northeast Normal University, Changchun, Jilin, 130024, P. R. China

E-mail: jpeng@nenu.edu.cn

^b Department of Chemistry, Bohai University, Jinzhou, Liaoning, 121000, P. R. China

Table S1. Selected bond lengths (Å) and angles (°) of compounds **1** and **2**.

Compound 1			
Ag(1)-N(10)	2.099(11)	Ag(3)#3-N(1)	2.264(10)
Ag(1)-N(11)	2.101(15)	Ag(3)-N(2)	2.237(9)
Ag(2)-N(12)	2.215(11)	Ag(4)#2-N(9)	2.564(13)
Ag(2)-N(8)	2.267(10)	Ag(4)-N(5)	2.580(13)
Ag(2)#2-N(6)	2.203(10)	Ag(4)-O(1W)	2.07(5)
Ag(3)#3-N(7)	2.336(10)	Ag(4)-N(9)#2	2.564(13)
N(10)-Ag(1)-N(11)	175.4(6)	N(2)-Ag(3)-N(7)#3	112.4(3)
N(6)#2-Ag(2)-N(12)	131.1(4)	N(1)#3-Ag(3)-N(7)#3	110.7(3)
N(6)#2-Ag(2)-N(8)	115.0(4)	O(1W)-Ag(4)-N(9)#2	80.2(8)
N(12)-Ag(2)-N(8)	110.7(4)	O(1W)-Ag(4)-N(5)	142.0(10)
N(2)-Ag(3)-N(1)#3	134.3(3)	N(9)#2-Ag(4)-N(5)	123.0(5)
Symmetry transformations used to generate equivalent atoms for 1: #2 -x+2,-y-1,-z+1; #3 -x+1,-y-1,-z+1.			
Compound 2			
Ag(1)-N(2)	2.102(10)	Ag(4)-N(7)	2.126(9)
Ag(1)-N(10)	2.148(8)	Ag(4)-N(4)	2.172(9)
Ag(2)-N(13)#1	2.116(8)	Ag(4)-O(21)	2.546(7)
Ag(2)-N(14)	2.135(9)	Ag(5)-N(8)	2.222(9)
Ag(3)-N(1)	2.140(9)	Ag(5)-O(20)	2.423(7)
Ag(3)-N(9)	2.147(8)	N(2)-Ag(1)-N(10)	166.8(4)
N(13)#1-Ag(2)-N(14)	175.4(3)	N(7)-Ag(4)-O(21)	98.2(3)
N(1)-Ag(3)-N(9)	163.3(4)	N(4)-Ag(4)-O(21)	80.6(3)
N(7)-Ag(4)-N(4)	174.5(3)	N(8)-Ag(5)-O(20)	141.5(3)
Symmetry transformations used to generate equivalent atoms for 2: #1 x-1,y-1,z+1.			

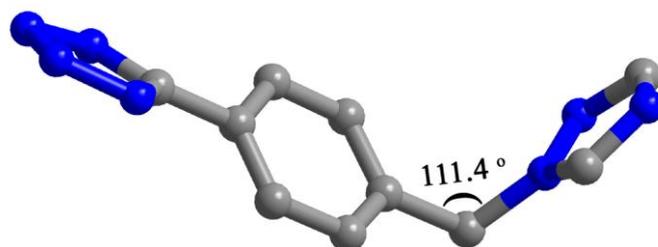


Fig. S1 The coordination configuration of the L₂ ligand in compound 2.

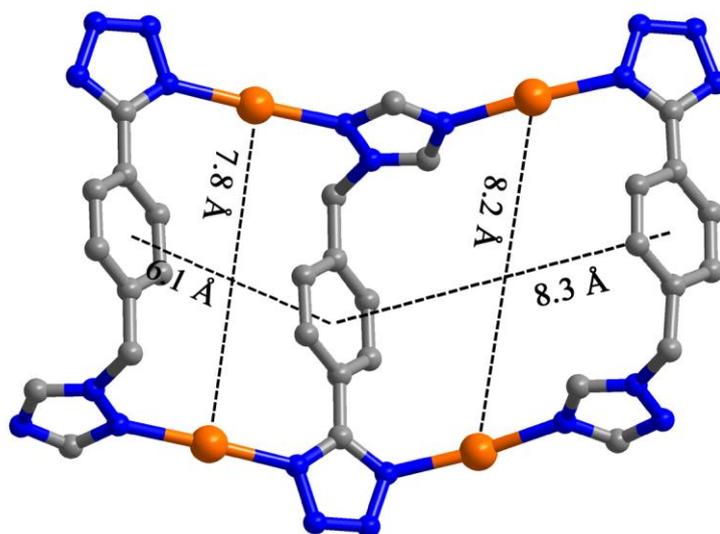


Fig. S2 View of the circles in compound 2.

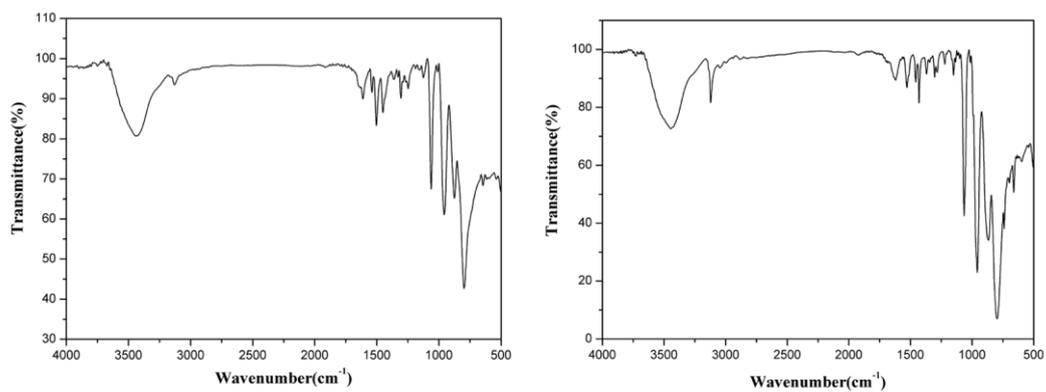


Fig. S3 The IR spectrums of compounds 1(left) and 2(right).

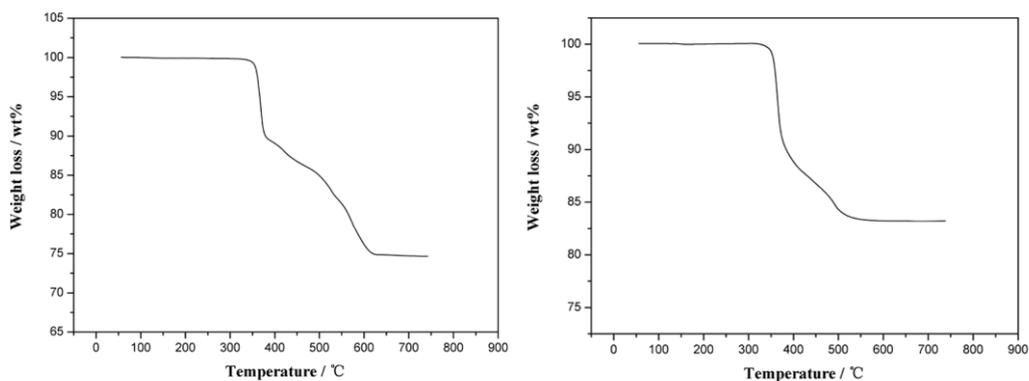


Fig. S4 TG curves of compounds **1**(left) and **2**(right).

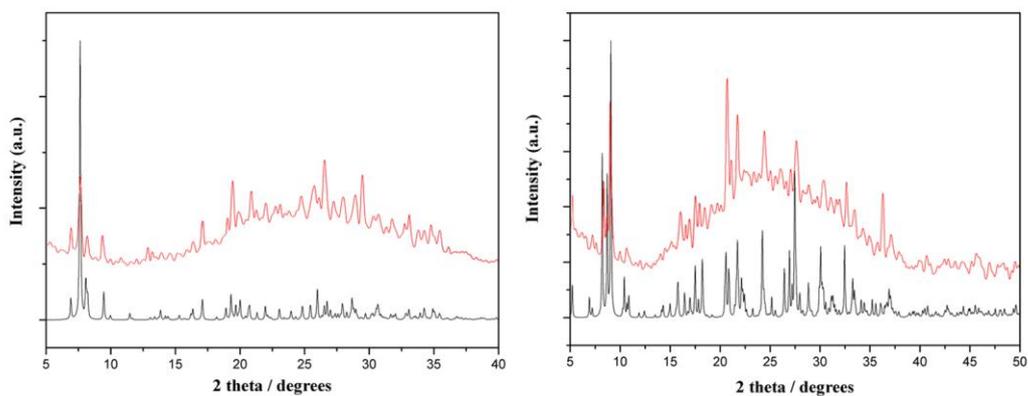


Fig. S5 The PXRD patterns for compounds **1**(left) and **2**(right).