Supporting Information

Ag(I)-based high-energy metal organic frameworks (HE-MOFs) incorporating the coordinated moieties in channels: Synthesis, structure and physicochemical properties

Xiaxia Song,^{#[a]} Sheng Zhang,^{#[a,b]} Guowei Zhao,^[a] Wendou Zhang,^[a] Dongpo Chen,^[a] Qi Yang,^{*[a]} Qing Wei,^[a] Gang Xie,^[a] Desuo Yang,^[b] Sanping Chen,^{*[a]} Shengli Gao^[a]

^{a.} Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi'an, Shaanxi 710127, P.R. China. E-mail: <u>yangqi@nwu.edu.cn</u>, <u>sanpingchen@126.com</u>

[#]These authors contributed equally to this work.

Ag(1)-N(5)	2.219(7)	Ag(1)-N(3)	2.246(7)
Ag(1)-O(2)	2.591(7)	Ag(1)-O(4)	2.613(7)
Ag(2)-N(12)	2.187(7)	Ag(2)-N(12)#1	2.187(7)
C(8)-O(4)#2	1.260(9)	N(1)-N(1)#3	1.291(13)
N(5)-Ag(1)-O(2)	117.5(3)	N(3)-Ag(1)-O(2)	87.5(2)
O(2)-Ag(1)-O(4)	75.7(2)	N(12)-Ag(2)-N(12)#1	180.0(3)
N(4)-N(3)-Ag(1)	122.5(5)	C(1)-N(3)-Ag(1)	129.7(7)
C(3)-N(5)-Ag(1)	131.2(7)	N(6)-N(5)-Ag(1)	120.6(5)
N(11)-N(12)-	117 8(5)	$C(6) \mathbb{N}(12) \mathbb{A}_{2}(2)$	121 5(6)
Ag(2)	117.8(3)	C(0) - N(12) - Ag(2)	131.3(0)
N(13)-O(2)-Ag(1)	102.8(5)	C(8)-O(4)-Ag(1)	111.3(5)

Table S1. Selected bond lengths (Å) and angles (°) for 1.

Symmetry transformations used to generate equivalent atoms for 1:

#1 -x,-y,-z; #2 -x+1,y,-z+1/2; #3 -x+3/2,-y+3/2,-z+1.

^{b.} College of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, Baoji 721013, P.R. China



Figure S1. X-ray powder diffraction pattern of 1.