

Electronic Supporting Information (ESI)

Syntheses, Structures and Magnetic Properties of Two Heterometallic Carbonates: $K_2Li[Cu(H_2O)_2Ru_2(CO_3)_4X_2] \cdot 5H_2O$ (X = Cl, Br)

Yan-Yan Jia,^a Bin Liu,^{a,*} Xue-Mei Liu,^a and Jian-Hui Yang,^{a,*}

^aKey Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry & Materials Science, Shaanxi Key Laboratory of Physico-Inorganic Chemistry, Northwest University, Xi'an 710069, P. R. China

Corresponding Author: liubin@nwu.edu.cn (B. Liu). yjhzj@yahoo.com (J. H. Yang).

Fax: +86-29-88302604.

Table S1. Selected bond angles (°) of complexes **1** and **2**

1			
Ru(1A)–Ru(1)–Cl(1)	177.35(11)	O(3)–Cu(1)–O(4)	92.9(2)
Ru(1A)–Ru(1)–O(1)	88.94(17)	O(4)–Cu(1)–O(3D)	87.1(2)
Ru(1A)–Ru(1)–O(2A)	90.48(17)	O(3)–Cu(1)–O(3E)	93.0(4)
Cu(2)–O(3)–C(1)	128.9(6)	O(3)–Cu(1)–O(3F)	87.0(4)

2			
Ru(1A)–Ru(1)–Br(1)	177.37(2)	O(5)–Cu(1)–O(6)	92.10(12)
Ru(1A)–Ru(1)–O(1A)	89.07(8)	O(5)–Cu(1)–O(7)	86.04(13)
Ru(1A)–Ru(1)–O(2)	90.36(8)	O5–Cu(1)–O6D	87.90(12)
Ru(1A)–Ru(1)–O(3A)	90.42(8)	O5–Cu(1)–O7D	93.96(13)
Ru(1A)–Ru(1)–O(4)	88.83(8)	O6–Cu1–O7D	89.52(12)
Cu(1)–O(5)–C(1)	130.3(3)	O6D–Cu1–O7D	90.48(12)
Cu(1)–O(6)–C(2A)	128.0(3)		

Symmetry codes: **1**: A : -x + 1, -y + 1, -z + 2; B: y, x, z; C : -y + 1, -x + 1, -z + 2; D: -x + 1, -y + 2, -z + 2; E: -y + 3/2, -x + 3/2, z; F: y -1/2, x + 1/2, -z + 2. **2**: A, 1/2 - x, 1/2 - y, z; D: -x, 1 - y, 1 - z.

* Corresponding author. Tel./fax: +86-029-88302604.

E-mail address: liubin@nwu.edu.cn (B. Liu)

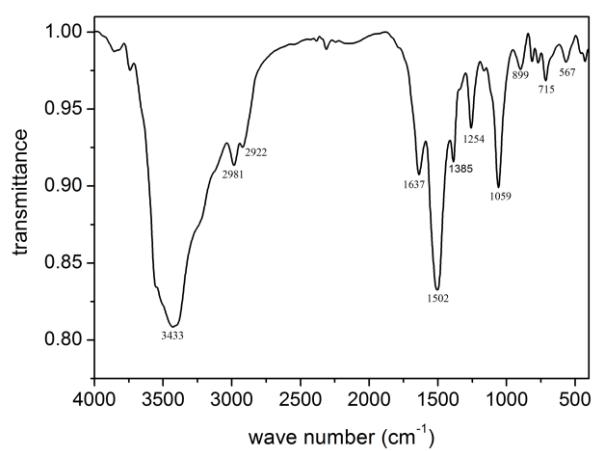


Fig S1. IR spectra of complex **1**.

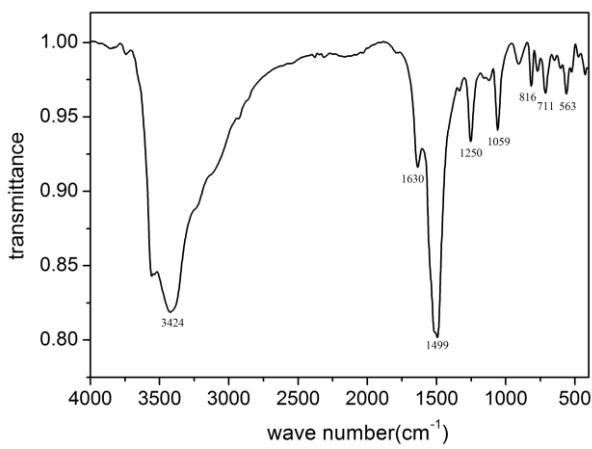


Fig S2. IR spectra of complex **2**.

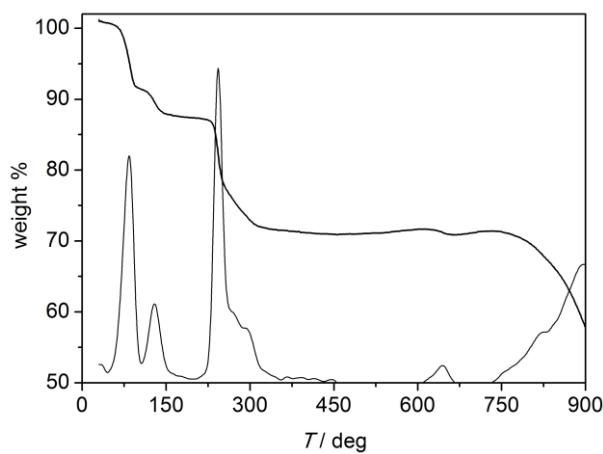


Fig S3. Themal analysis of complex **1**.

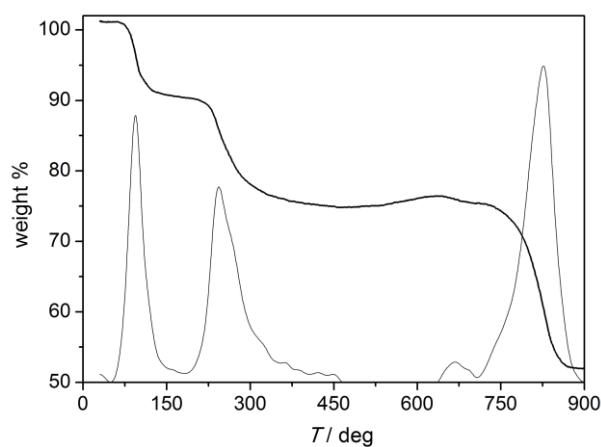


Fig S4. Themal analysis of complex **2**.

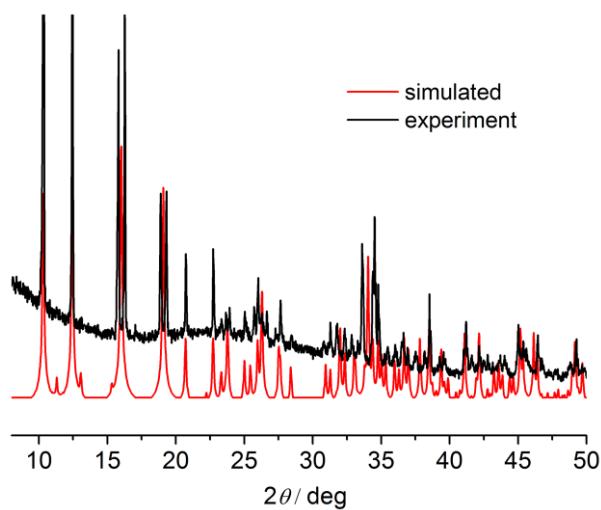


Fig. S5 Comparison of XRPD patterns of the simulated and as-synthesized of **1**.

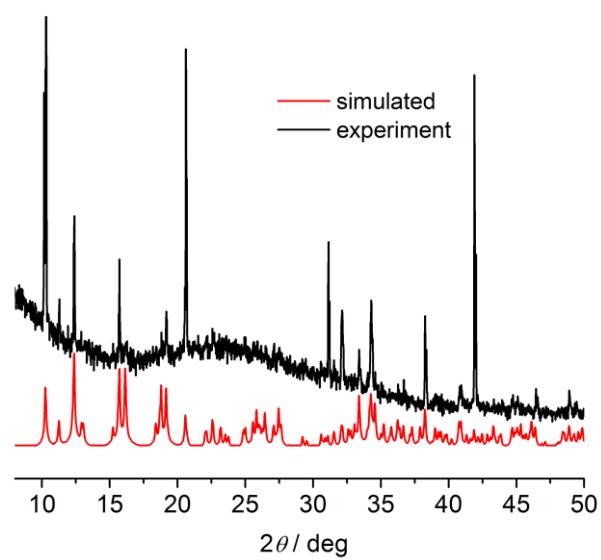


Fig. S6 Comparison of XRPD patterns of the simulated and as-synthesized of **2**.

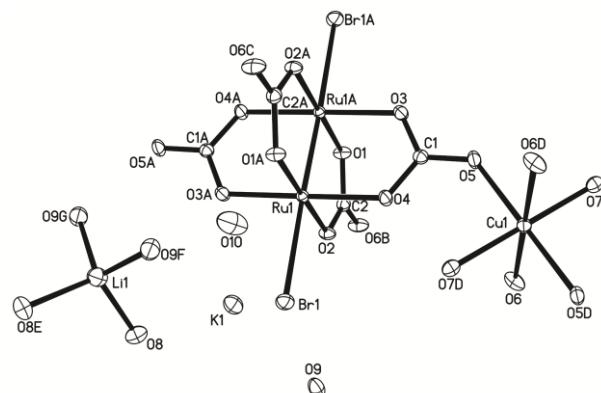


Fig. S7 ORTEP representation (30% thermal probability ellipsoids) of the crystal structure of **2**

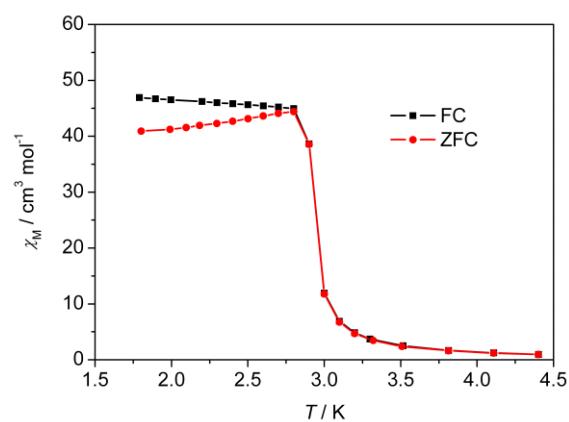


Fig. S8 FC and ZFC vs T plots for complex **1**.

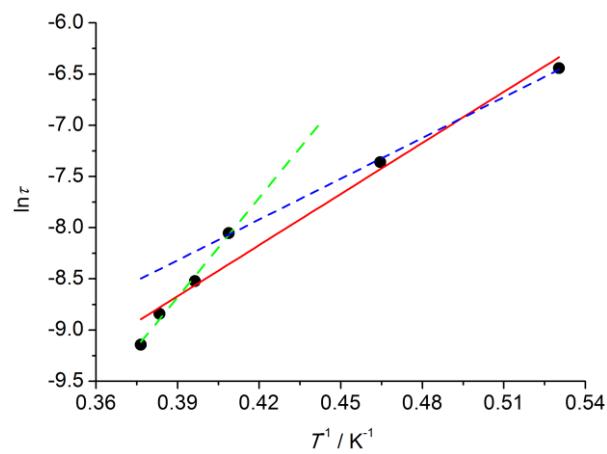


Fig. S9 The Arrhenius plots and best linear fits for complex **1**.

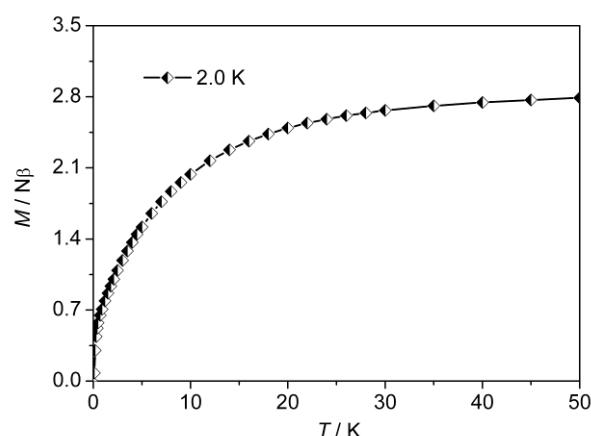


Fig. S10 M vs H plot for complex 2

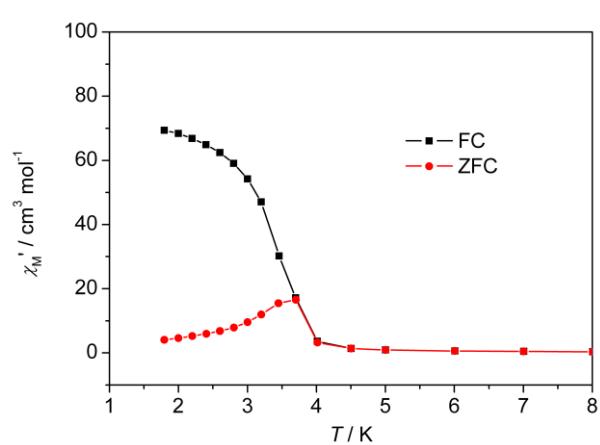


Fig. S11 FC and ZFC vs T plots for 2