Supporting Information

Structures, Magnetic and Catalytic Properties of Three Sandwich-Type Silicotungstates Containing Tetranuclear Copper(II) Clusters

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Thermogravimetric analysis of 1, 2 and 3

Thermogravimetric analysis (TGA) studies were performed in a N₂ atmosphere at a heating rate of 10 °C/min⁻¹ for complexes **1-3**. As shown in Fig.S1, the TGA diagram of **1** displays the weight loss of 11.5 % between room temperature and 400°C, which correspond to the removal of 22 guest water molecules, 12 NH₃ and 2 aqua molecules (calcd 11.8%). Between 400 and 900°C, **1** shows no weight loss. Similary, the TGA curves of **2** and **3** display the weight loss of 10.3 % (calcd 8.7 % for **2**) and 11.4% (calcd. 10.0 % for **3**) respectively, which correspond to the loss of all the NH₃ and H₂O molecules.

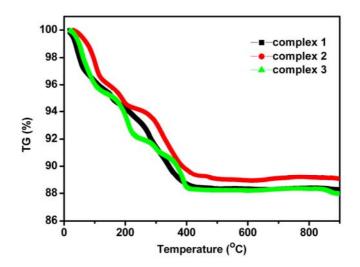


Fig. S1 TGA curve for 1-3 over temperature range of 20-900 °C.

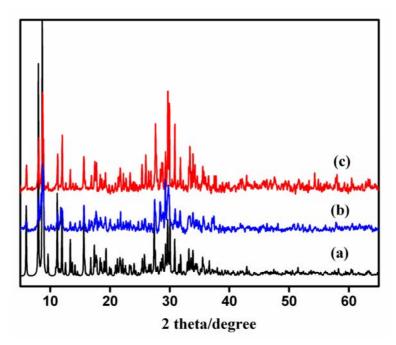


Fig. S2 XRPD patterns of **1** (a) simulation based on the single-crystal structure; (b) the synthesized **1** at 298 K, (c) after reaction for 10 h at 343 K.

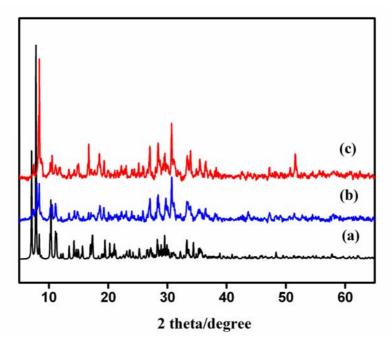


Fig. S3 XRPD patterns of **2** (a) simulation based on the single-crystal structure; (b) the synthesized **2** at 298 K, (c) after reaction for 10 h at 343 K.

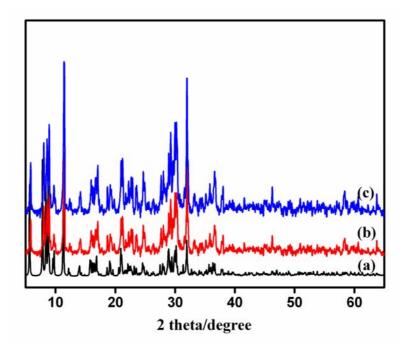


Fig. S4 XRPD patterns of **3** (a) simulation based on the single-crystal structure; (b) the synthesized **3** at 298 K, (c) after reaction for 10 h at 343 K.

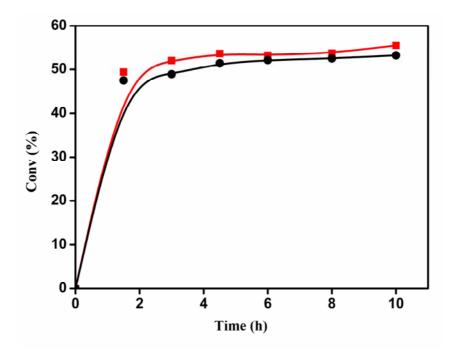


Fig. S5 Reaction condition: ethylbenzene (0.3 mL, 2.44 mmol), catalyst (0.01 mmol), 70% TBHP (0.75 mL, 4.88 mmol), acetonitrile (8 mL) (■): fresh catalyst; (●): recycle for one time.