

Fig. s1. The ball-and-stick and wire representation of the hydrogen bonds in compound 2.

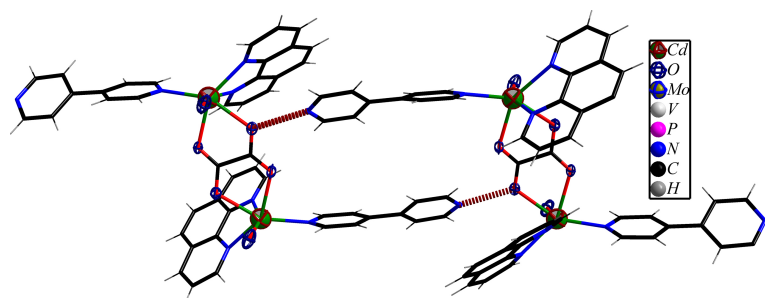


Fig. s2. The wire representation of the 1-D supramolecular chain constructed from the CTMCs in compound 3.

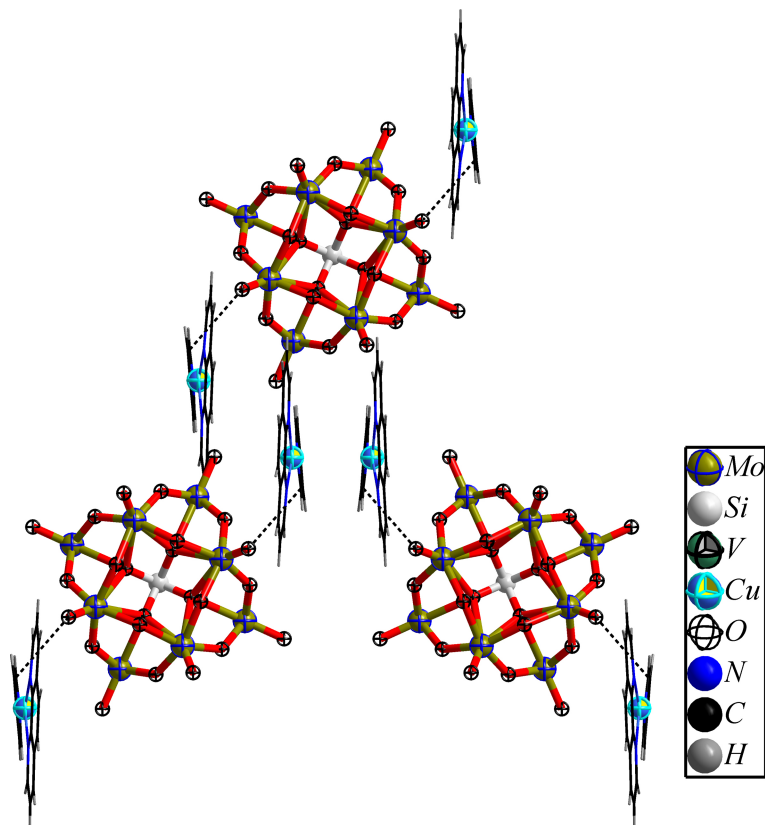


Fig. s3. The representation of  $\pi \cdots \pi$  interactions in compound 5.

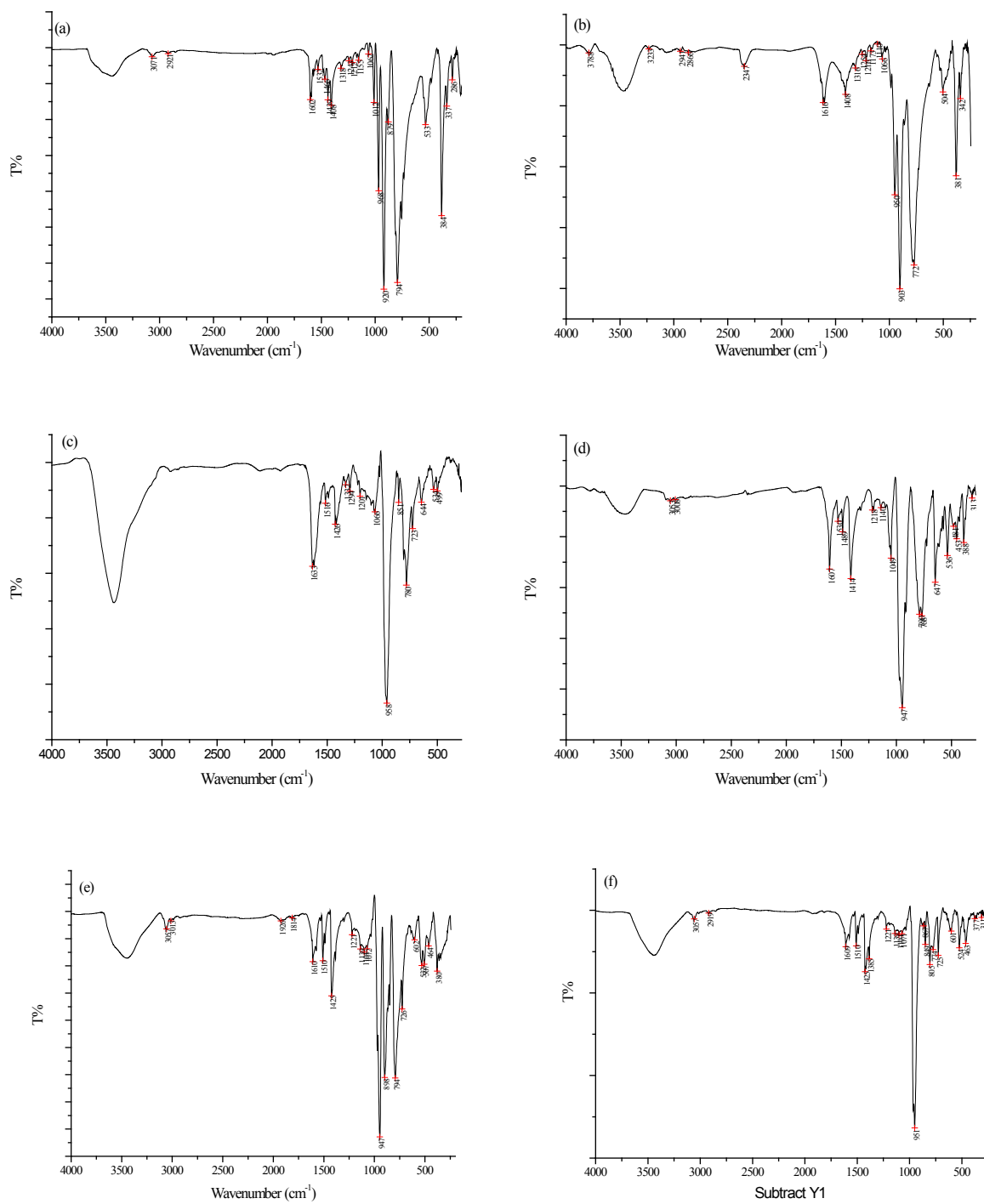


Fig. s4. The IR spectra for compound 1 (a), compound 2 (b), compound 3 (c), compound 4 (d), compound 5(e) and compound 6(f).

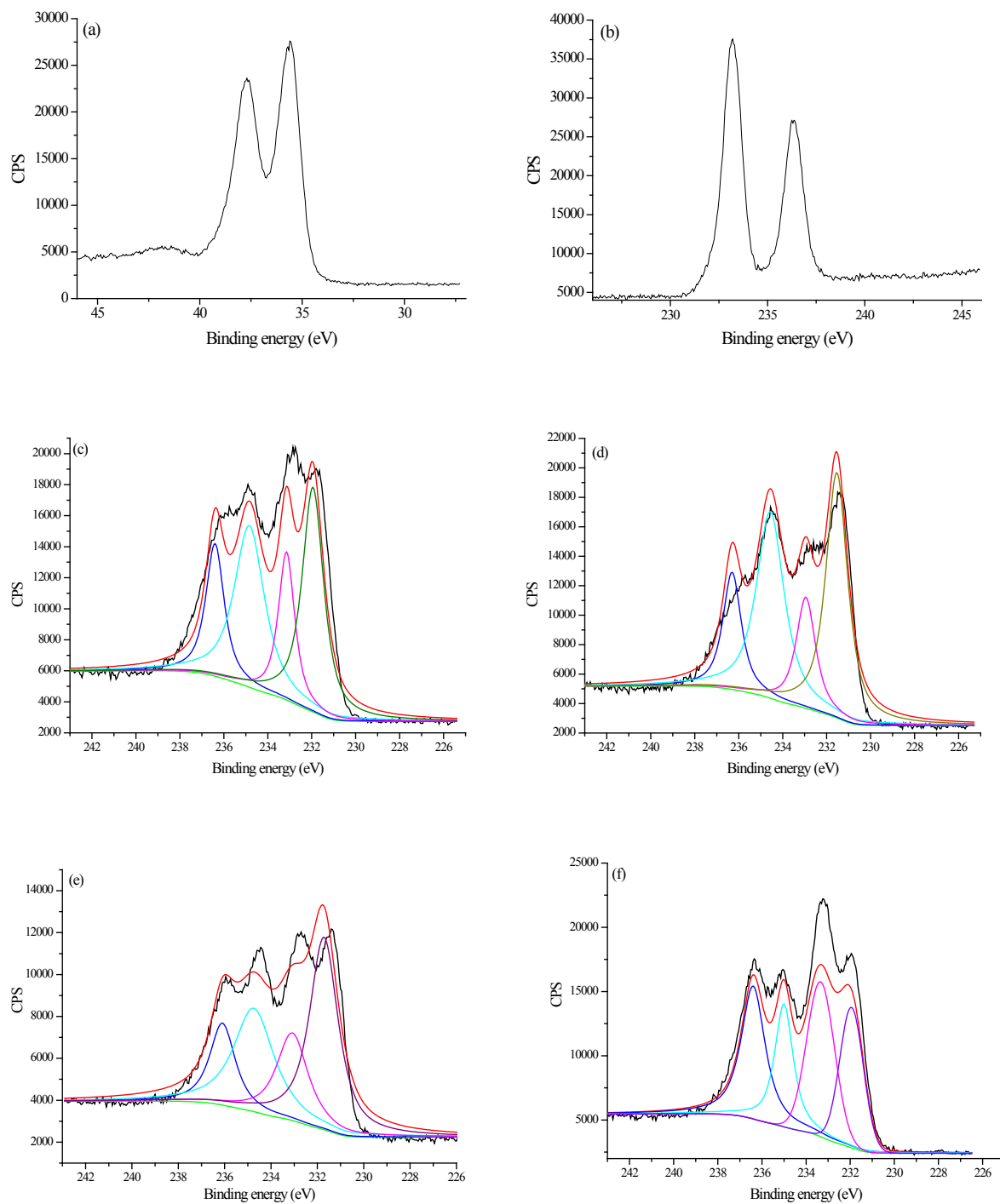
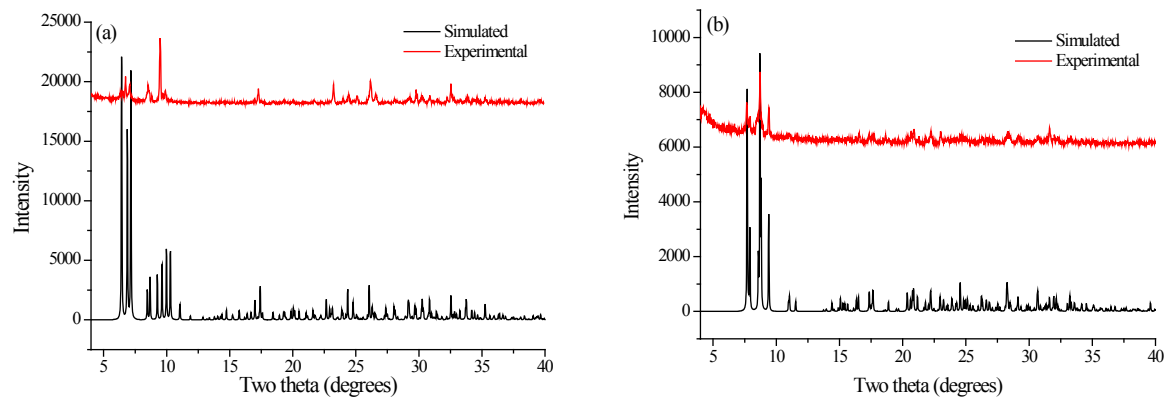


Fig. s5. The XPS spectrum for tungsten in compound 1 (a) and the XPS spectra for molybdenum in compound 2 (b), compound 3 (c), compound 4 (d), compound 5(e) and compound 6(f).



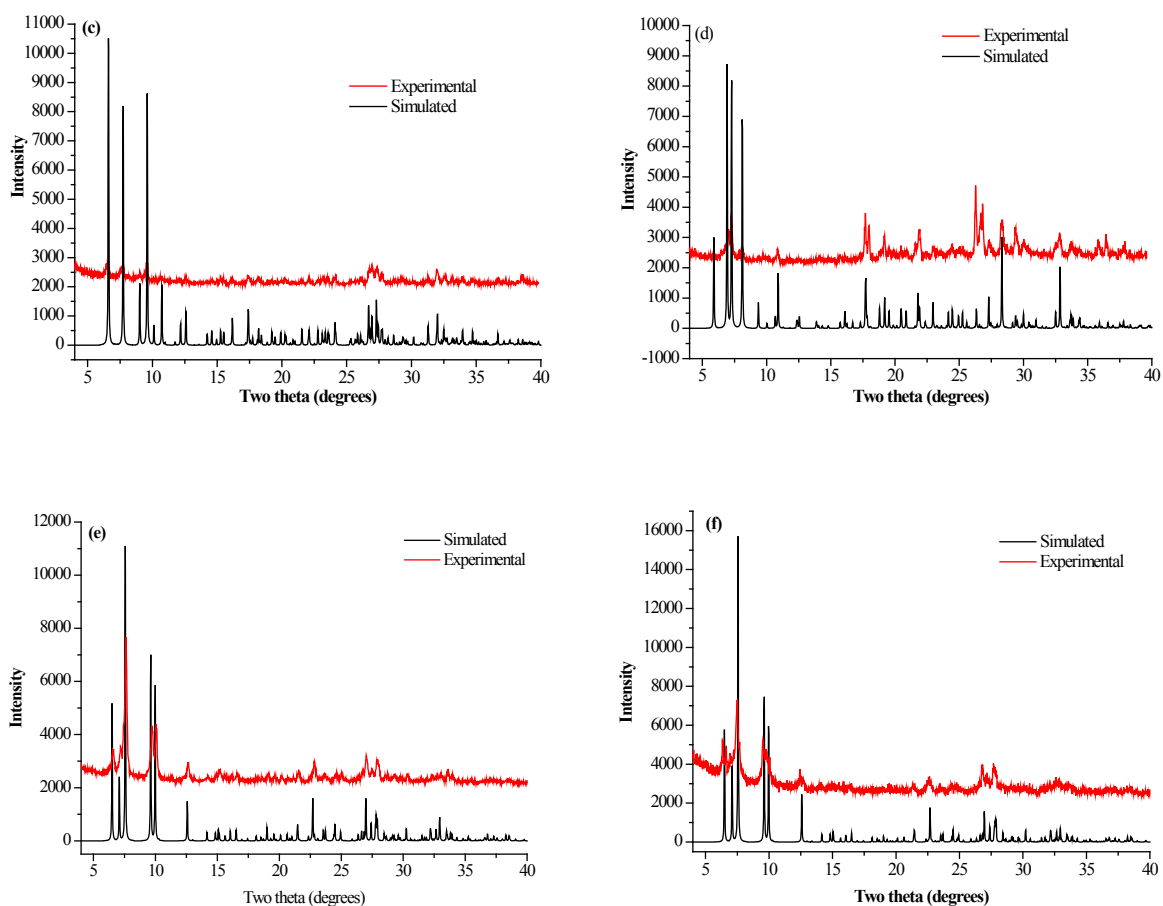
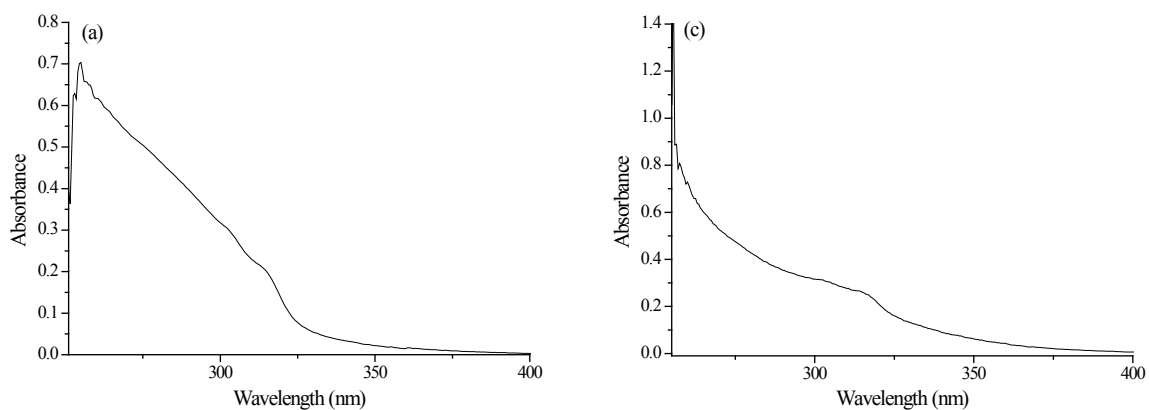


Fig. S6. (a) The experimental and simulated XRD pattern for compound **1**; (b) The experimental and simulated XRD pattern for compound **2**; (c) The experimental and simulated XRD pattern for compound **3**; (e) The experimental and simulated XRD pattern for compound **5**; (f) The experimental and simulated XRD pattern for compound **6**.



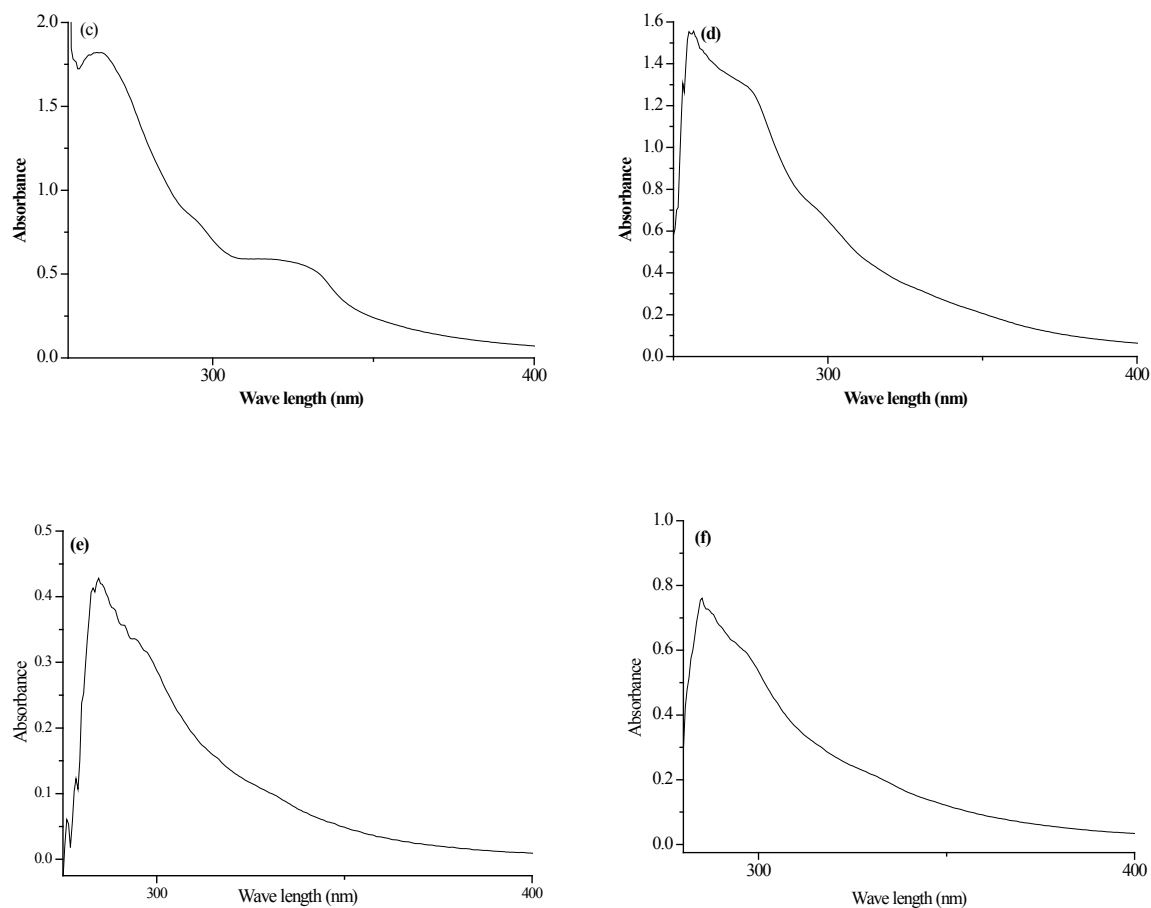
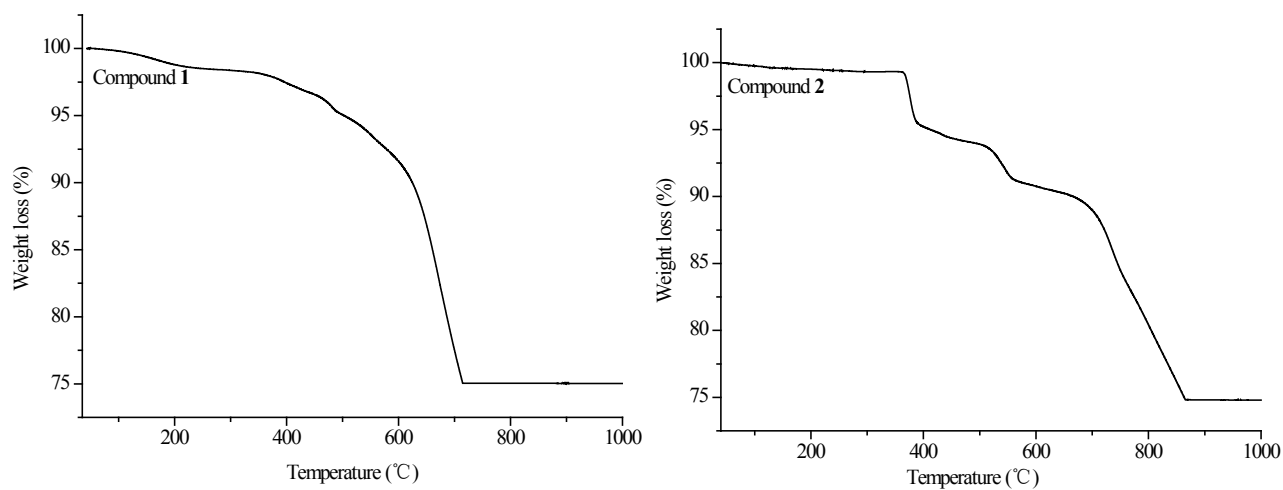


Fig. S7. The UV-Vis spectrum for compound **1** (a), compound **2** (b), compound **3** (c), compound **4** (d), compound **5** (e) and compound **6** (f).



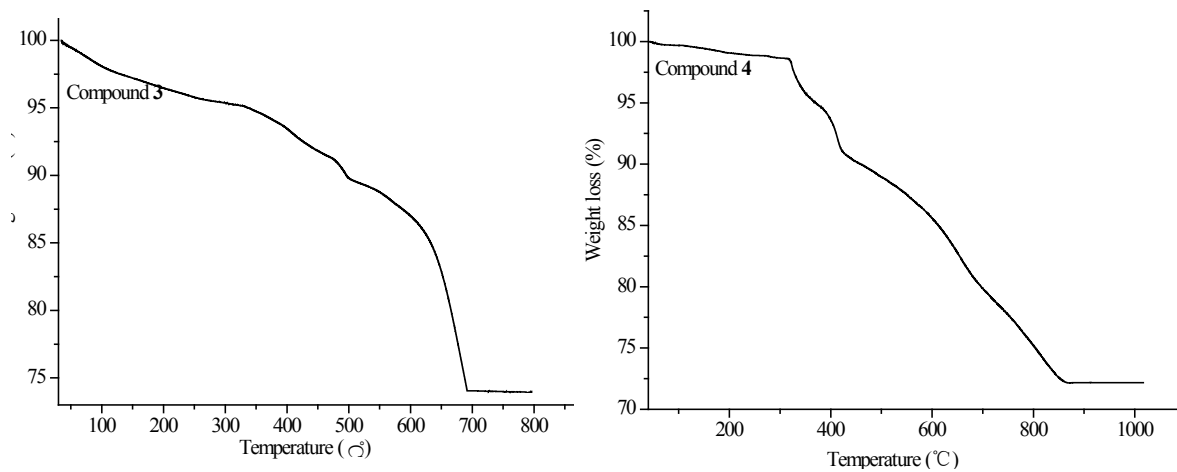


Fig. s8 the TG curves of compound 1-4.