Supplementary Material

Towards applications in catalysis: Investigation on photocatalytic activities of a derivative family of the Kepelerate type molybdenum-oxide based polyoxometalate

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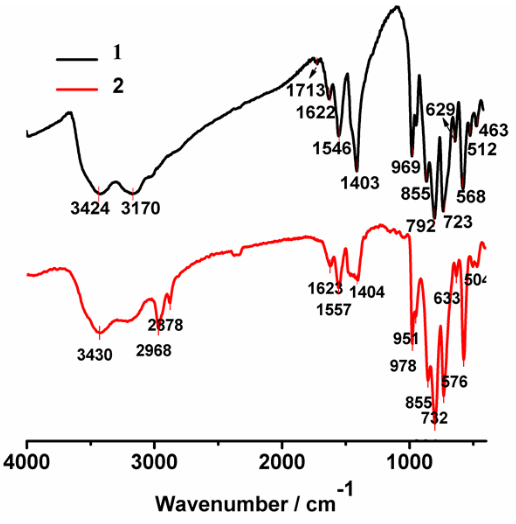

Fig. S1. IR of compounds **1** (reference to: A. Müller, E. Krickemeyer, H. Bögge, M. Schmidtmann, F. Peters, *Angew. Chem. Int. Ed.* **1998**, *37*, 3359-3363) and **2** (reference to: Y. Zhou, Z. Shi, L. Zhang, S. Hassan and N. Qu, *Appl. Phys. A: Mater. Sci. Process.* **2013**, *113*, 563-568)

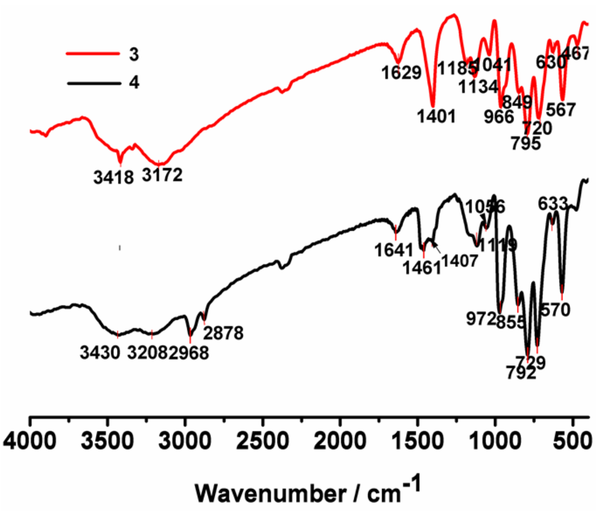

Fig. S2. IR spectra of compounds **3** and **4**

It can be seen that the characteristic bands (Fig. S2) ascribed to the $[\mathrm{Mo}^{VI}_{72}\mathrm{Mo}^{V}_{60}\mathrm{O}_{372}(\mathrm{SO}_4)_{30}(\mathrm{H}_2\mathrm{O})_{72}]^{72-}$ anion are nearly remained after formation of the compound **4** derived from the compound **3**（reference to: A. Müller, E. Krickemeyer, H. Bögge, M. Schmidtmann, B. Botar, M. O. Talismanova, *Angew. Chem. Int. Ed.* **2003**, *42*, 2085-2090), indicating that the structure of the anion in is kept and remained in the compound **4**, while the notable appearance of the middle-strong bands at 2968 (ν_{as}(C-H)) and 2878 (ν_s(C-H)) cm^{-1} confirms the presence of the $\mathrm{Bu}_4\mathrm{N}^+$ cations in the compound **4**. The broad band in the range of 3450~3000 cm^{-1} centered at 3439 and 3208 cm^{-1} in **4** corresponds to the O-H stretching vibrations of crystallization water molecules.

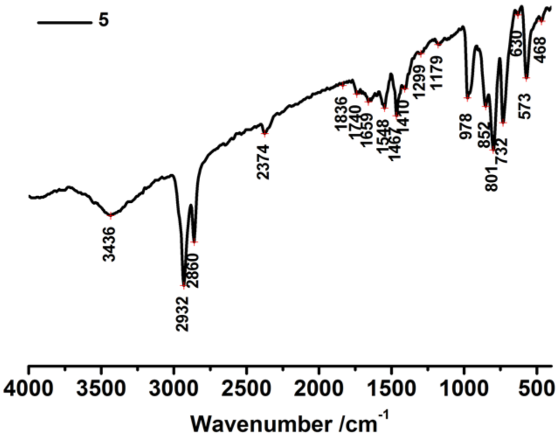

Fig. S3. IR spectra of compound **5** (reference to: D. Volkmer, D. G. Kurth, H. Schnablegger, P. Lehmann, M. J. Koop, A. Müller, *J. Am. Chem. Soc.* **2000**, *122*, 1995-1998)

Thermogravimetric analysis of compound 4

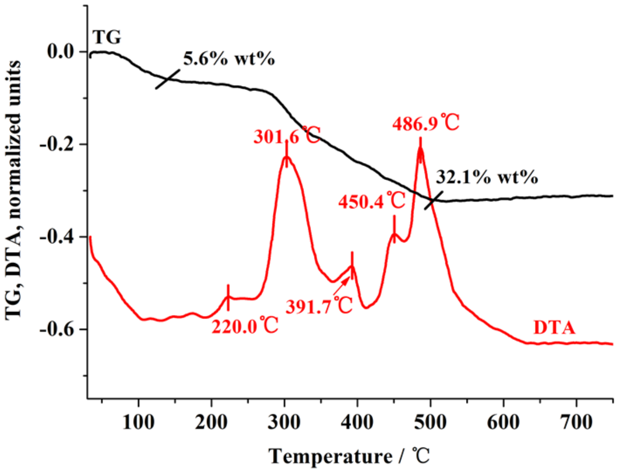

Fig. S4. The TG and DTA spectra for compound **4**

As shown in Fig. S4, the weight loss process of compound **4** can be divided into two steps. The first step is from 35 ℃ to 115℃ with a weight loss of 5.6%, corresponding to the release of 110 lattice water molecules (calcd. 5.8%), with two corresponding exothermal peak at 43.23 °C in DTA curve. The second weight loss (26.5%) between 115 ℃ and 750 ℃ is attributed to the loss of 44 NH_3, 100 lattice water molecules, 72 coordinated water molecules and the decomposition of organic components (calcd 25.6%), leading to the formation of corresponding $[(n\text{-Bu})_4N]_8[Mo^{VI}_{72}Mo^{V}_{60}O_{372}(SO_4)_{30}(H_2O)_{72}]$, with a few main corresponding exothermal peak at 220.0, 301.6, 391.7, 450.4 and 486.9 °C in DTA curve.

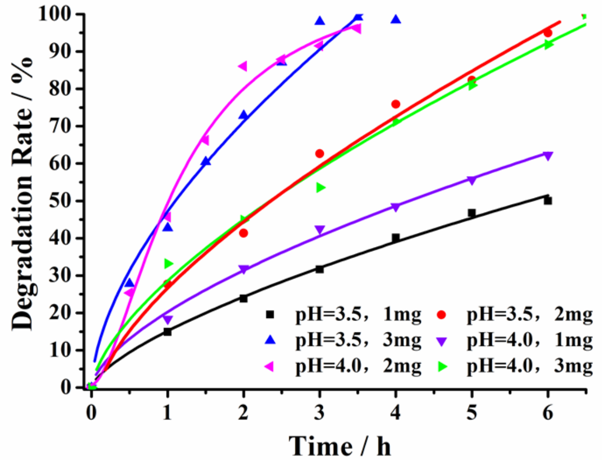

Fig. S5. Dosage effects of compound **2** from 1 ~ 3 mg when the initial pH of RhB solution was 3.5 and 4.0, respectively. Reaction condition: 50 ml of 2 mg/L RhB solution.

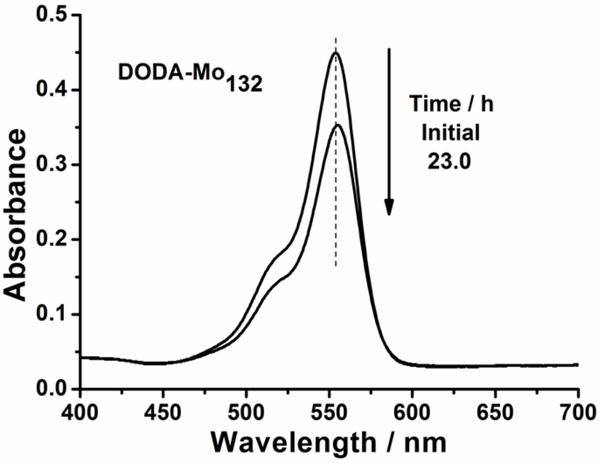

Fig. S6. UV-vis spectral changes of RhB during the catalytic process with compound **5** as catalyst. Reaction condition: 50 ml of 2 mg/L RhB solution, pH 3.5, 2 mg of compound **5**

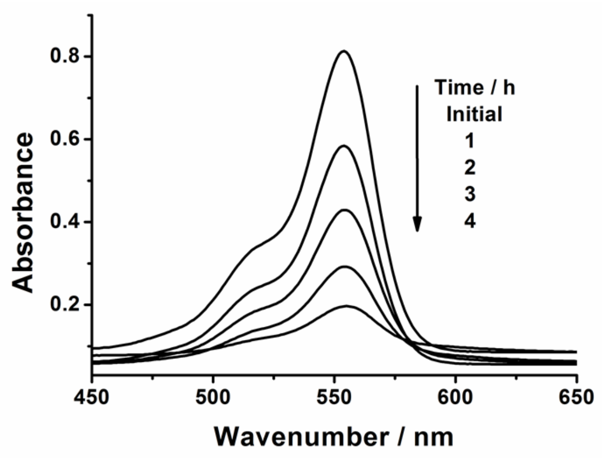

Fig. S7. UV-vis spectral changes of RhB during the catalytic process with commercial TiO_2 as catalyst. The arrow marks the increase of reaction time. Reaction condition: 50 ml of 2 mg/L RhB solution, pH 3.5, 2 mg of TiO_2.

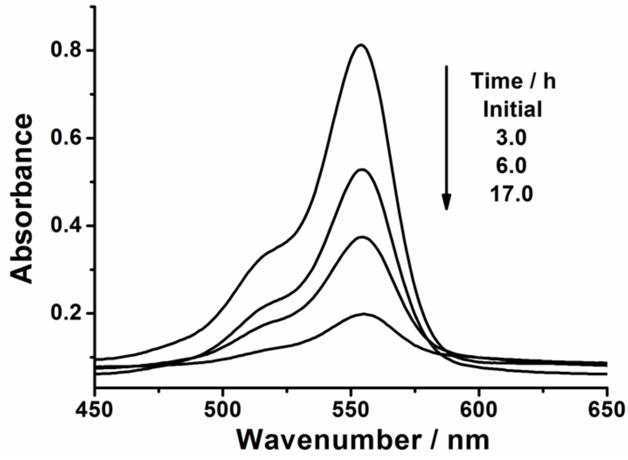

Fig. S8. UV-vis spectral changes of RhB during the catalytic process with compound **4** as catalyst. The arrow marks the increase of reaction time. Reaction condition: 50 ml of 2 mg/L RhB solution, pH 3.5, 2 mg of compound **4**.

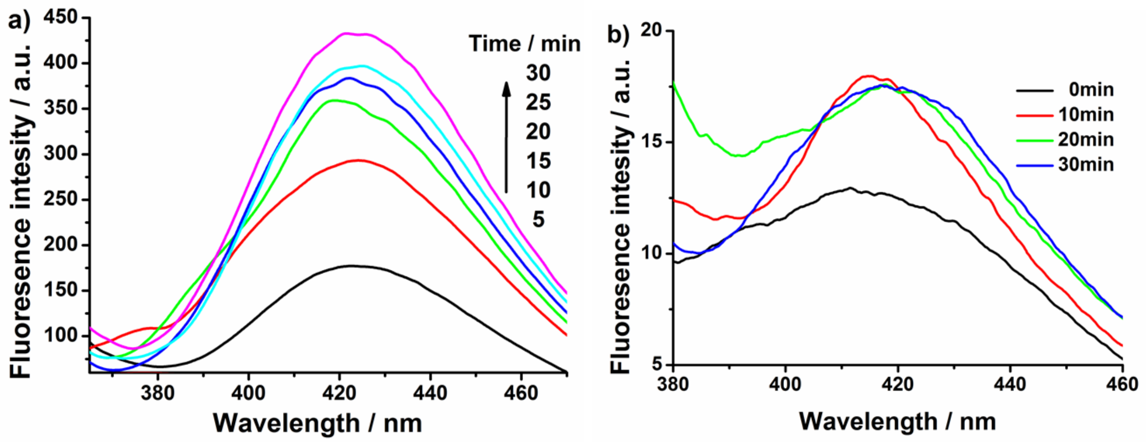

Fig. S9. Photoluminescence spectral changes (λ_{max} = 425 nm) versus UV light irradiation time for compounds **4** (a) and **5** (b) in a 5 × 10^{-4} mol·L^{-1} basic solution of terephthalic acid (excitation light λ = 315 nm, Voltage = 500V, EX slit = 10 nm, EM slit = 10 nm).

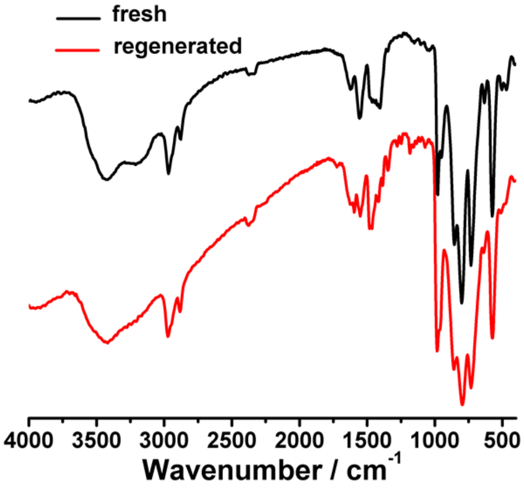

Fig. S10 IR spectra of fresh and regenerated compound **2**.