

# Supporting Information

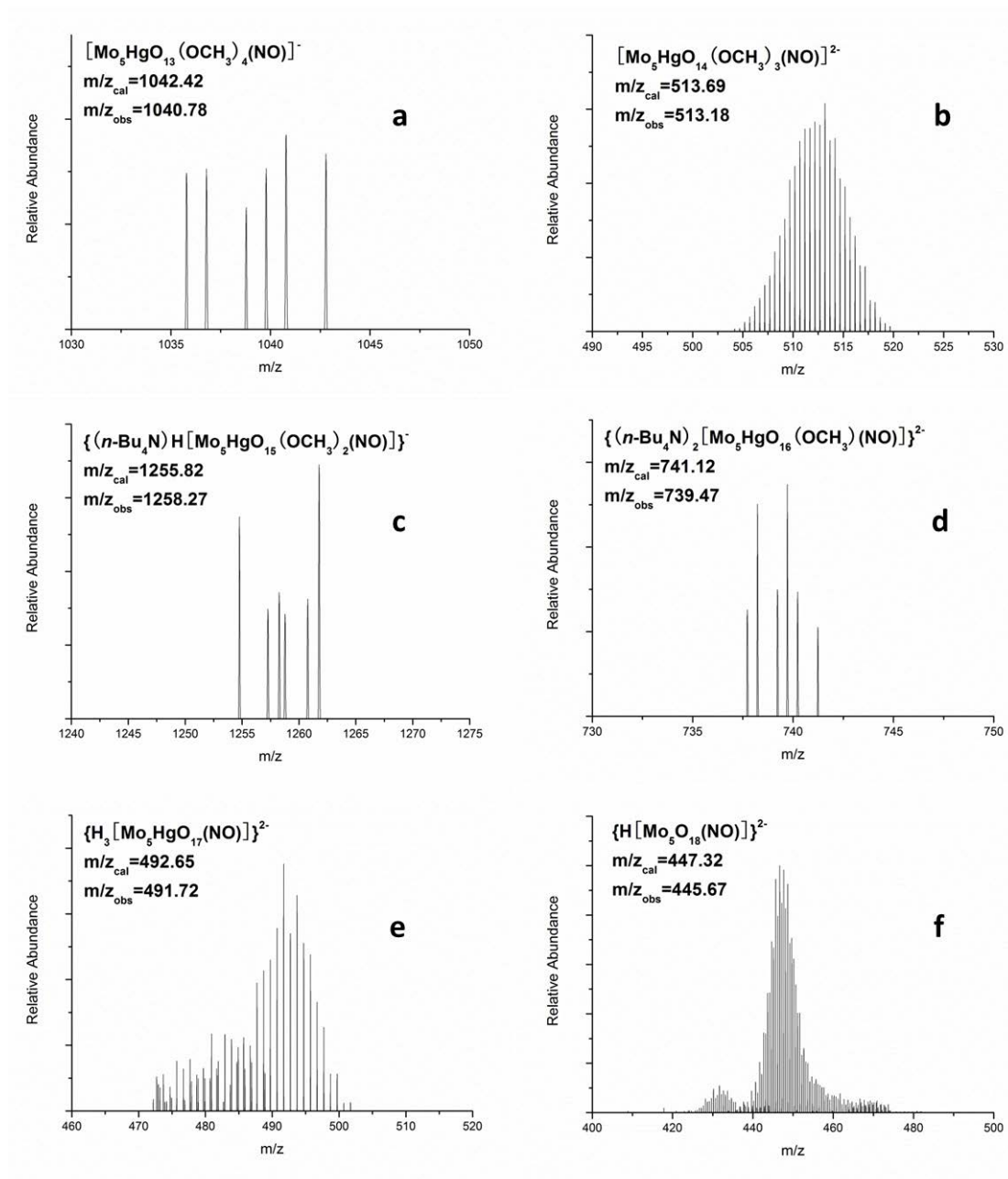
## Label-free colorimetric detection of mercury via $\text{Hg}^{2+}$ ions-accelerated structural transformation of nanoscale metal-oxo clusters

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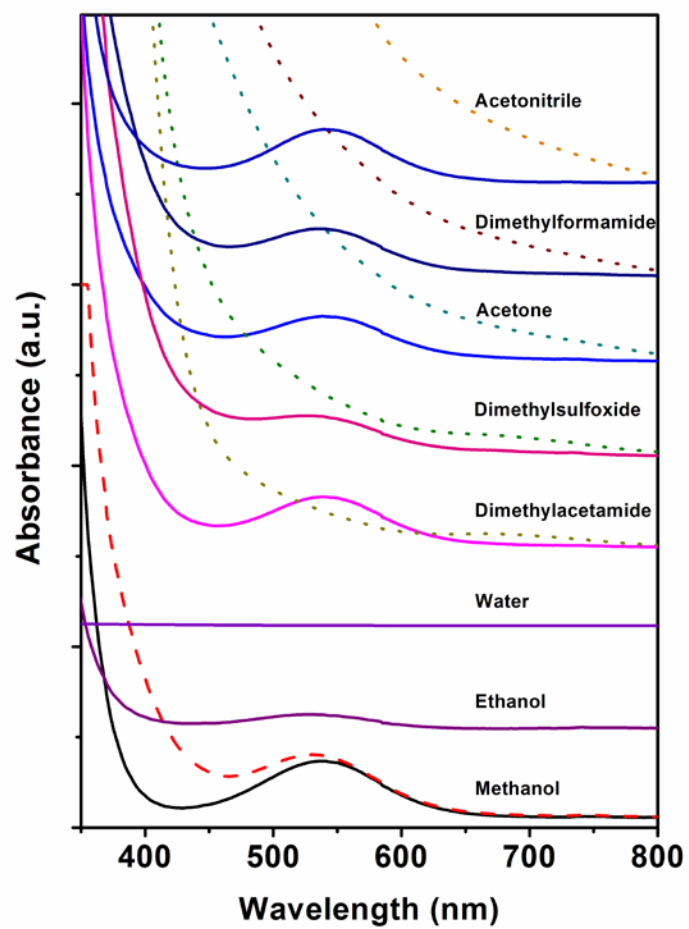
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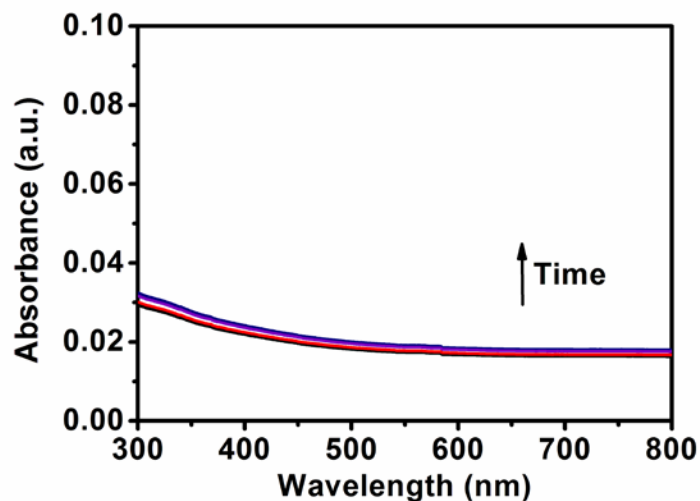
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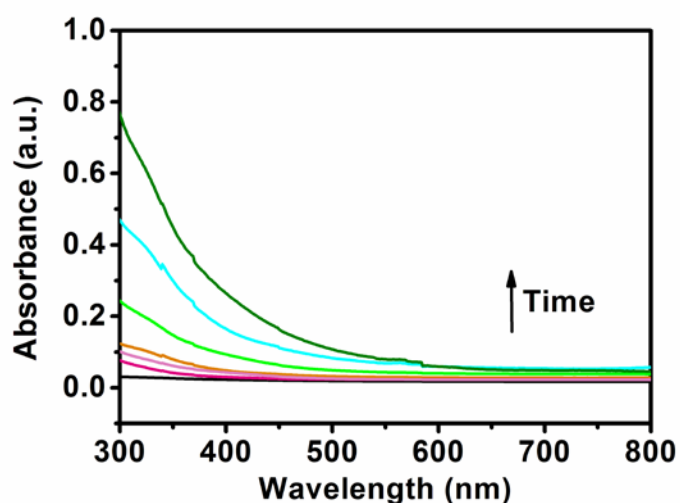
**Figure S1.** ESI-MS spectra of probably intermediate products:  $[\text{Mo}_5\text{HgO}_{13}(\text{OCH}_3)_4(\text{NO})]^-$  (a),  $[\text{Mo}_5\text{HgO}_{14}(\text{OCH}_3)_3(\text{NO})]^{2-}$  (b),  $[\text{Mo}_5\text{HgO}_{15}(\text{OCH}_3)_2(\text{NO})]^{3-}$  (c),  $[\text{Mo}_5\text{HgO}_{16}(\text{OCH}_3)(\text{NO})]^{4-}$  (d),  $[\text{Mo}_5\text{HgO}_{17}(\text{NO})]^{5-}$  (e), and product  $[\text{Mo}_6\text{O}_{18}(\text{NO})]^{3-}$  (f).



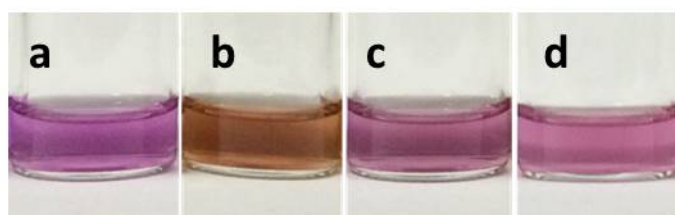
**Figure S2.** UV-vis spectra of MLPOM in different solvent. Absorbance of MLPOM in methanol (in the presence (red dash line) or absence (black line) of Hg<sup>2+</sup>), water, ethanol, and other organic solvent: dimethylacetamide, dimethylsulfoxide, acetone, dimethylformamide and acetonitrile (recorded immediately (full line) and 3d later (dot line)).



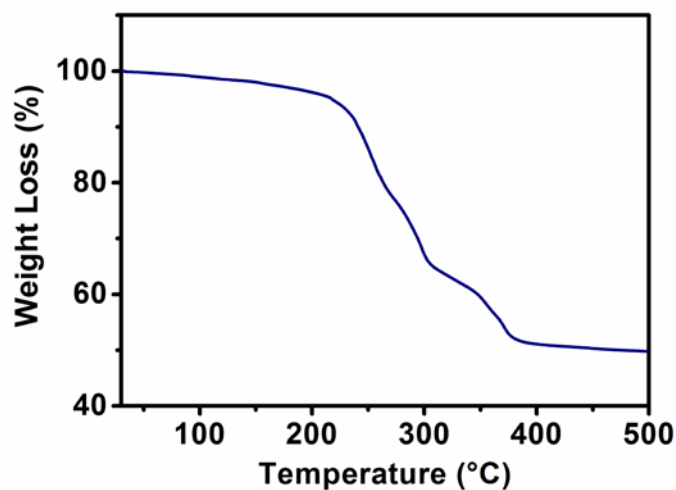
**Figure S3.** UV-vis spectra of MLPOM in water at different time point. From the bottom up: 10 min (blank), 30 min (red), 60 min (purple), 120 min (navy). Low absorbance is due to the low solubility of MLPOM in water.



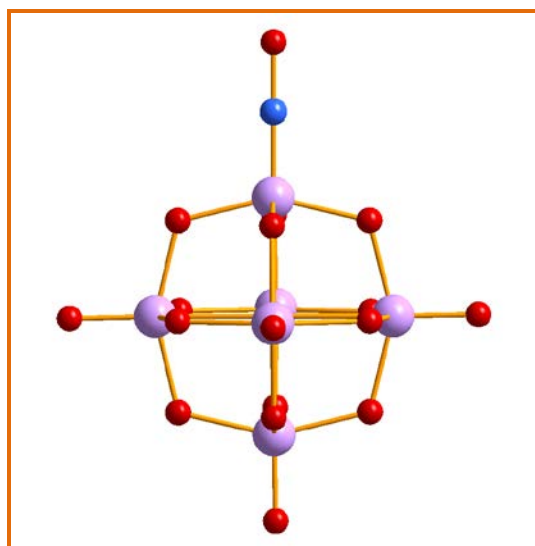
**Figure S4.** UV-vis spectra of MLPOM in water at different time point under heating of 80 °C. From the bottom up: 0 min (blank), 5 min (red), 10 min (magenta), 15 min (orange), 20 min (green), 25 min (cyan), 30 min (olive).



**Figure S5.** Photographs of MLPOM solution (a), in the presence of  $\text{Hg}^{2+}$  (b), after adding hydroxylamine hydrochloride (c), and  $[\text{Mo}_6\text{O}_{18}(\text{NO})]^{3-}$  after re-dispersing in methanol (d).



**Figure S6.** Thermo gravimetric (TG) curve of  $(n\text{-Bu}_4\text{N})_2[\text{Mo}_5\text{NaO}_{13}(\text{OCH}_3)_4(\text{NO})]$  at a heating rate of  $10\text{ }^\circ\text{C}/\text{min}$  under Ar atmosphere.



**Figure S7.** Ball-and-stick representation of  $[\text{Mo}_6\text{O}_{18}(\text{NO})]^{3-}$  anion: Mo, light purple; O, red; N, blue.

## References

1. Gouzerh, P., Jeannin, Y., Proust, A., Robert, F. Two novel polyoxomolybdates containing the  $(\text{MoNO})^{3+}$  unit:  $[\text{Mo}_5\text{Na}(\text{NO})\text{O}_{13}(\text{OCH}_3)_4]^{2-}$  and  $[\text{Mo}_6(\text{NO})\text{O}_{18}]^{3-}$ . *Angew. Chem., Int. Ed.* **28**, 1363 (1989).
2. Proust, A., Gouzerh, P., Robert, F. Molybdenum oxo nitrosyl complexes. 1. Defect Lindqvist compounds of the type  $[\text{Mo}_5\text{O}_{13}(\text{OR})_4(\text{NO})]^{3-}$  ( $\text{R} = \text{CH}_3, \text{C}_2\text{H}_5$ ). Solid-state interactions with alkali-metal cations. *Inorg. Chem.* **32**, 5291 (1993).