## **Supporting Information**

## N-Heterocycle Chelated Oxomolybdenum(VI and V) Complexes with Bidentate Citrate

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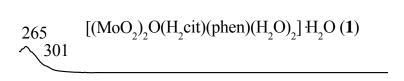
## **Experimental Section**

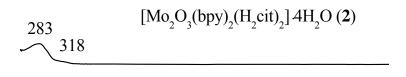
Physical Measurements

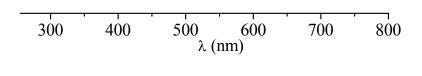
Infrared spectra were recorded as Nujol mulls between KBr plates with a Nicolet 360 FT-IR spectrometer. Electronic spectra in solution were recorded on a UV 2501 spectrophotometer. Elemental analyses were performed with an EA 1110 elemental analyzer. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded in DMSO on a Bruker 400 NMR spectrometer using DSS (sodium 2,2-dimethyl-2-silapentane-5-sulfonate) as the internal reference.

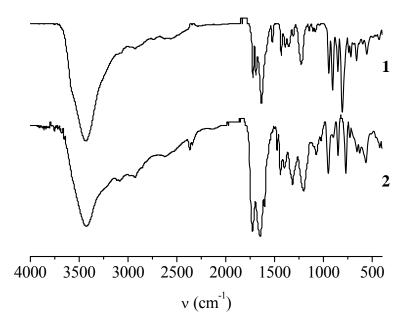
## **Figure Options**

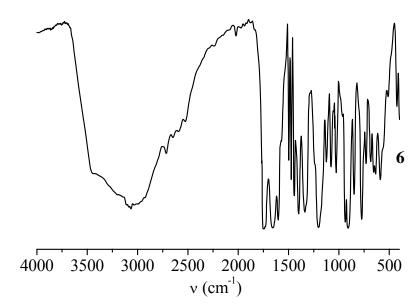
- Figure S1 UV-Vis spectra of  $[(MoO_2)_2O(H_2cit)(phen)(H_2O)_2]\cdot H_2O$  (1) and  $[(MoO)_2O(H_2cit)_2(bpy)_2]\cdot 4H_2O$  (2) in DMSO solution Figure S2 IR spectra of  $[(MoO_2)_2O(H_2cit)(phen)(H_2O)_2]\cdot H_2O$  (1) and
- Figure S2 IR spectra of  $[(MoO_2)_2O(H_2cit)(phen)(H_2O)_2]\cdot H_2O(1)$  and  $[(MoO)_2O(H_2cit)_2(bpy)_2]\cdot 4H_2O(2)$
- Figure S3 IR spectra of  $[MoO_2(H_2cit)(bpy)] \cdot H_2O(6)$
- Figure S4 Calculated and experimental X-ray diffractogram of  $[(MoO_2)_2O(H_2cit)(phen)(H_2O)_2]\cdot H_2O~(\textbf{1}).$
- Figure S5 The <sup>13</sup>C NMR data of the solution of sodium molybdate(VI) and citric acid with the molar ratio Mo:cit = 1:1 at various pH values in equilibrium. \* denotes dimeric molybdenum citrate, o denotes monomeric molybdenum citrate, x denotes free citrate.

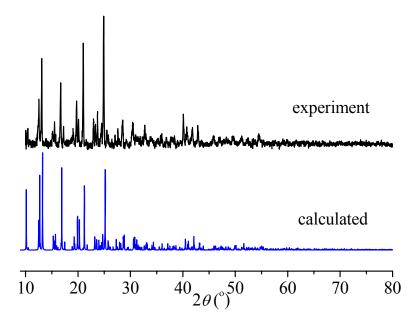




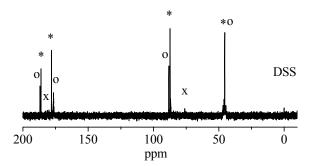




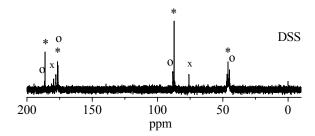




Mo :
$$H_4$$
cit = 1 : 1  
pH = 0.5



Mo :
$$H_4$$
cit = 1 : 1  
pH = 1.0



Mo :
$$H_4$$
cit = 1 : 1  
pH = 2.0

