# 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. ${ }^{1} \mathrm{H}$ and ${ }^{13} \mathrm{C}$ NMR spectra were recorded in DMSO on a Bruker 400 NMR spectrometer using DSS (sodium 2,2-dimethyl-2-silapentane-5sulfonate) as the internal reference.

## Figure Options

Figure S1 UV-Vis spectra of $\left[\left(\mathrm{MoO}_{2}\right)_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{cit}\right)(\mathrm{phen})\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right] \cdot \mathrm{H}_{2} \mathrm{O}(\mathbf{1})$ and $\left[(\mathrm{MoO})_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{cit}\right)_{2}(\mathrm{bpy})_{2}\right] \cdot 4 \mathrm{H}_{2} \mathrm{O}(2)$ in DMSO solution

Figure S2 IR spectra of $\left[\left(\mathrm{MoO}_{2}\right)_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{cit}\right)(\mathrm{phen})\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right] \cdot \mathrm{H}_{2} \mathrm{O}(\mathbf{1})$ and $\left[(\mathrm{MoO})_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{cit}\right)_{2}(\text { bpy })_{2}\right] \cdot 4 \mathrm{H}_{2} \mathrm{O}(\mathbf{2})$

Figure S3 IR spectra of $\left[\mathrm{MoO}_{2}\left(\mathrm{H}_{2} \mathrm{cit}\right)(\right.$ bpy $\left.)\right] \cdot \mathrm{H}_{2} \mathrm{O}(\mathbf{6})$

Figure S4 Calculated and experimental X-ray diffractogram of $\left[\left(\mathrm{MoO}_{2}\right)_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{cit}\right)(\right.$ phen $\left.)\left(\mathrm{H}_{2} \mathrm{O}\right)_{2}\right] \cdot \mathrm{H}_{2} \mathrm{O}(\mathbf{1})$.

Figure S5 The ${ }^{13} \mathrm{C}$ 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, $\circ$ denotes monomeric molybdenum citrate, x denotes free citrate.


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\left[\mathrm{Mo}_{2} \mathrm{O}_{3}(\mathrm{bpy})_{2}\left(\mathrm{H}_{2} \mathrm{cit}\right)_{2}\right] 4 \mathrm{H}_{2} \mathrm{O}(2)
$$

318

| 300 | 400 | 500 | 600 | 700 | 800 |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  | $\left.{ }^{1} \mathrm{~nm}\right)$ |  |  |  |

Figure S2


Figure S3



$\mathrm{Mo}: \mathrm{H}_{4} \mathrm{cit}=1: 1$
$\mathrm{pH}=1.0$


Mo $: \mathrm{H}_{4}$ cit $=1: 1$
$\mathrm{pH}=2.0$




