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**Fig. S1** X-ray molecular structures of (a) cis-[MoO<sub>2</sub>(acacL<sup>3</sup>)] (**3**) and (b) cis-[MoO<sub>2</sub>(acacL<sup>4</sup>)] (**4**) with the atom labeling schemes. In both structures, thermal ellipsoids of all non-hydrogen atoms are drawn at the 30% probability level.



(b)

**Fig. S2** Centrosymmetric N–H···O hydrogen bonded dimers of (a) cis-[MoO<sub>2</sub>(acacL<sup>3</sup>)] (**3**) and (b) cis-[MoO<sub>2</sub>(acacL<sup>4</sup>)] (**4**).



Fig. S3 Electronic spectra of 1–5 in methanol.



**Fig. S4** <sup>1</sup>H NMR spectra of 1-5 in dimethylsulfoxide-d<sub>6</sub>.



**Fig. S5**<sup>13</sup>C NMR spectra of **1–5** in dimethylsulfoxide-d<sub>6</sub>.