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Supporting Information

Molybdenum complexes having $\mu\text{-O}\{\text{MoO}_2\}_2$ core: Synthesis, crystal structure and application as catalyst for the oxidation of bicyclic alcohols using N-based additives

Mannar R. Maurya, Lata Rana and Fernando Avecilla

Table S1 IR Spectral data (in cm^{-1}) of the compounds

Compounds	$\nu(\text{OH})$	$\nu(\text{C}=\text{N})$	$\nu(\text{N}-\text{N})$	$\nu(\text{MoO}_2)$ asym.			$\nu(\text{Mo}-\text{O}-\text{Mo})$
$\text{H}_2\text{L}^1\text{I}$	3069	1592	974				
$\text{H}_2\text{L}^2\text{II}$	3075	1592	964				
$\text{H}_2\text{L}^3\text{III}$	3081	1591	963				
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^1)] \mathbf{1}$	3431	1549	995	950	915		773
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^2)] \mathbf{2}$	3428	1543	997	944	923		767
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^3)] \mathbf{3}$	3422	1542	991	933	889		769

Table S2 UV-vis spectral data of ligands and complexes

Compounds	$\lambda_{\text{max}}/\text{nm}$ ($\epsilon/\text{M}^{-1}\text{cm}^{-1}$)
$\text{H}_2\text{L}^1\text{I}$	297 (9720), 358 (11100)
$\text{H}_2\text{L}^2\text{II}$	298 (9320), 371 (10420)
$\text{H}_2\text{L}^3\text{III}$	308 (19400), 376 (13740)
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^1)] \mathbf{1}$	320 (5680), 363 (4760), 410 (2580)
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^2)] \mathbf{2}$	323 (6640), 371 (3100), 416 (3200)
$[(\mu\text{-O})\{\text{Mo}^{\text{VI}}\text{O}_2(\text{MeOH})\}_2(\text{L}^3)] \mathbf{3}$	320 (5720), 371 (3760), 410 (3180)

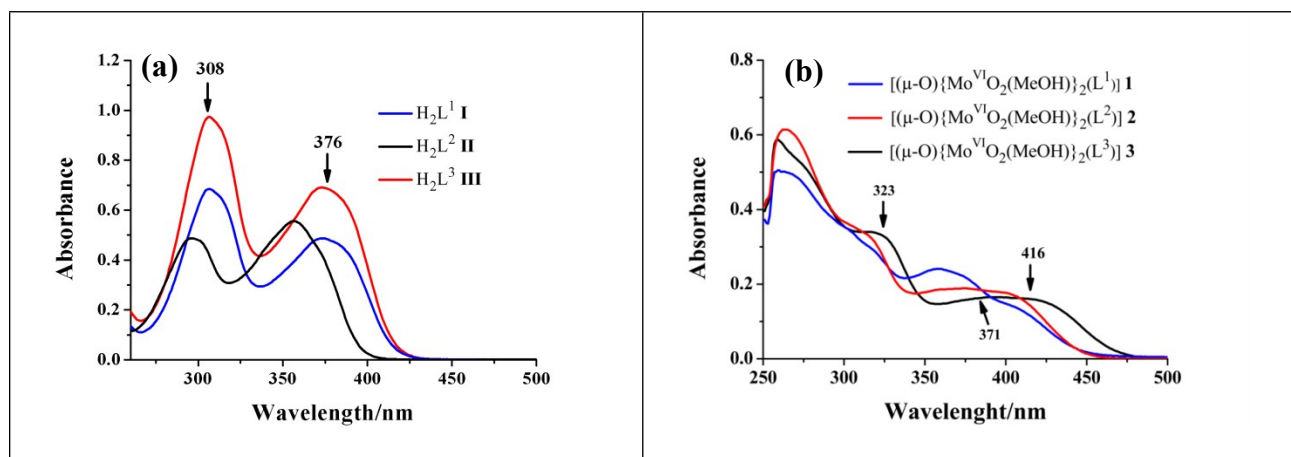


Fig. S1 UV-Vis spectra of (a) ligands and (b) complexes recorded in DMSO.

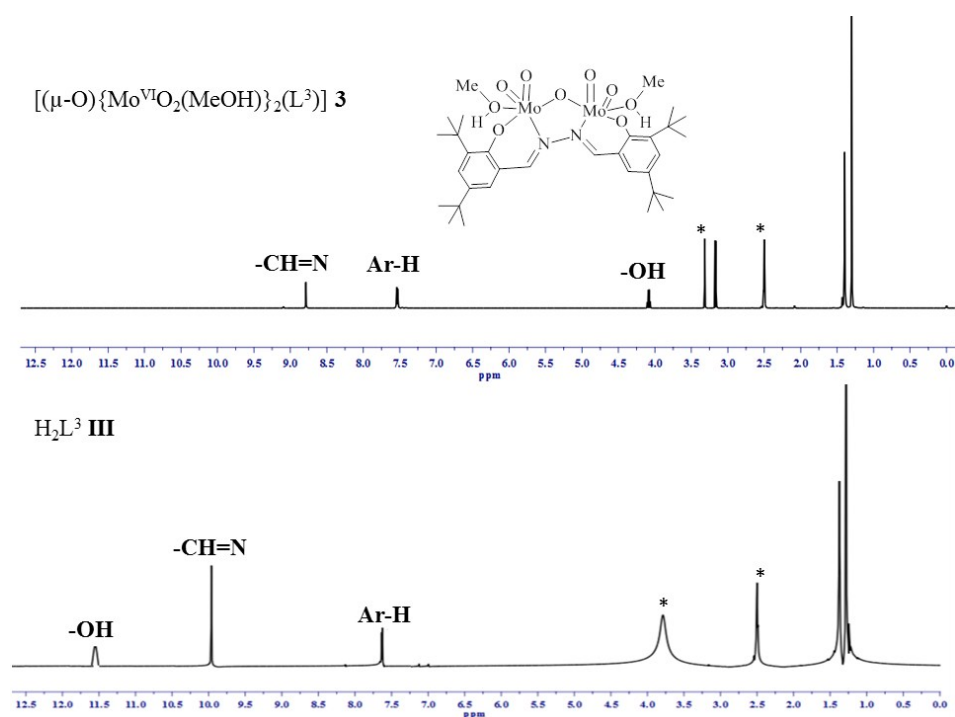


Fig. S2 ^1H NMR spectra of ligand $\text{H}_2\text{L}^3\text{III}$ and complex **3** recorded in DMSO-d_6 ; * indicates the proton impurity signal present in DMSO-d_6 at $\delta = 2.5$ ppm and that of moisture at $\delta = 3.5$ ppm.