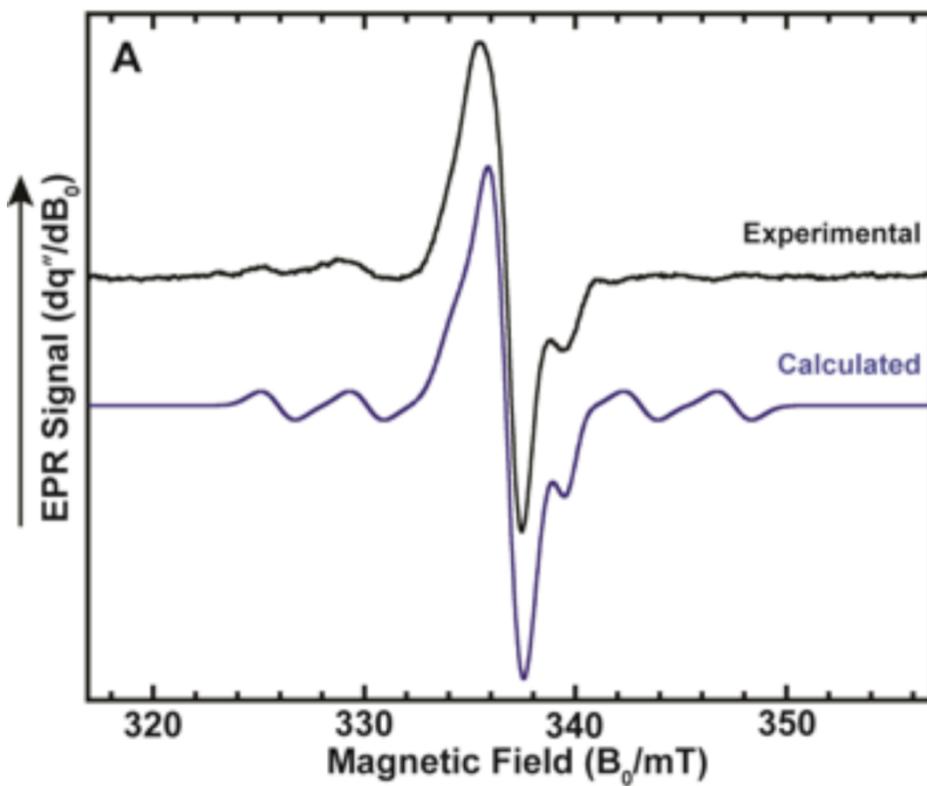


**Fig. S1** Change of absorbance of compound **II** in benzene solution ( $10^{-3}\text{M}$ ) in presence of  $10^{-2}\text{M}$  acetone. Three isosbestic points may be noted.



**Fig. S2** EPR spectrum (experimental) of compound **IIb** and its EasySpin simulated (calculated) spectrum. Calculated  $g_x$ ,  $g_y$  and  $g_z$  values ( $S = 1/2$ ) are 1.9987, 1.9999 and 2.0037 respectively. No hyperfine splitting due to  $^{14}\text{N}$  ( $S = 1$ ) could be observed because of large H-strain (anisotropic line broadening).  $H_x$ ,  $H_y$  and  $H_z$  values are  $\sim 50\text{MHz}$ ,  $50\text{MHz}$  and  $50\text{MHz}$ .

**Table S1** Crystal data and refinement details of three molybdenum complexes

	Compound IIa	Compound IIb	Compound IIc
Empirical formula	$\text{C}_{39}\text{H}_{36}\text{MoN}_6\text{O}_3\text{S}_3$	$\text{C}_{27}\text{H}_{27}\text{MoN}_6\text{O}_4\text{S}_3$	$\text{C}_{18}\text{H}_{20}\text{Mo}_2\text{N}_2\text{O}_9\text{S}_3$
Formula weight	828.86	691.67	696.42
Crystal system	Trigonal	Orthorhombic	Triclinic
Space group	P-3	$\text{P2}_1\text{2}_1\text{2}_1$	P1
Unit cell dimensions	$a = 13.6005(5)$ $b = 13.6005(5)$ $c = 11.9425(3)$ $\alpha = 90^\circ$ $\beta = 90^\circ$ $\gamma = 120^\circ$	$a = 7.7621(3)\text{\AA}$ $b = 31.6938(14)\text{\AA}$ $c = 12.9838(5)\text{\AA}$ $\alpha = \beta = \gamma = 90^\circ$	$a = 7.2719(4)\text{\AA}$ $b = 8.8902(7)\text{\AA}$ $c = 10.5788(7)\text{\AA}$ $\alpha = 68.497(7)^\circ$ $\beta = 87.429(5)^\circ$ $\gamma = 71.028(6)^\circ$
Cell volume $\text{\AA}^3$	1913.09(11)	3023(4)	599.59(7)
Z	2	4	1
Calculated density $\text{Mg m}^{-3}$	1.439	1.520	1.929
Absorption coefficient $\mu$	0.552	0.684	1.359
F(000)	852	1412	346
Theta range for data collection	2.43 to $30.00^\circ$	2.54 to $30.00^\circ$	2.61 to $29.99^\circ$

Reflections: Collected/ unique	13548/3725 [ $R_{\text{int}} = 0.0794$ ]	21445/8805 [ $R_{\text{int}} = 0.0646$ ]	4273/3361 [ $R_{\text{int}} = 0.0204$ ]
Crystal size (mm)	0.22 x 0.04 x 0.04	0.22 x 0.03 x 0.03	0.24 x 0.03 x 0.03
Completeness to theta	99.9	99.9	95.4
Max. and min. transmission	1.000 and 0.933	1.000 and 0.901	1.000 and 0.875
Data[ $I > 2\sigma(I)$ ]/Parameter	3026/161	6315/384	3008/167
Goodness of fit on $F^2$	1.013	1.027	0.762
Final R indices [ $I > 2\sigma(I)$ ]	$R_1 = 0.0423$ $wR_2 = 0.0888$	$R_1 = 0.0706$ , $wR_2 = 0.1716$	$R_1 = 0.0306$ $wR_2 = 0.0809$
R indices (all data)	$R_1 = 0.0582$ $wR_2 = 0.0970$	$R_1 = 0.0969$ , $wR_2 = 0.1801$	$R_1 = 0.0360$ $wR_2 = 0.0832$
Largest differential peak and hole ( $e \text{ \AA}^{-3}$ )	0.566 and -1.428	2.466 and -2.154	0.957 and -1.007