

SUPPLEMENTARY INFORMATION

Hemilability of phosphine-thioether ligands coordinated to trinuclear Mo₃S₄ clusters and its effect on hydrogenation catalysis

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Figure S3. Left: ESI-MS of brown solution after filtration of green [1]PF₆. Right: Simulated isotopic distribution.

Figure S4. ³¹P {¹H} NMR spectra of [3]PF₆: before adding of Bu₄NCl (up); after three hours of reaction with Bu₄NCl (down).

Figure S5. ESI-MS of [Mo₃S₄Cl₃(PS)₃]⁺ species after reaction of nitrobenzene reduction.

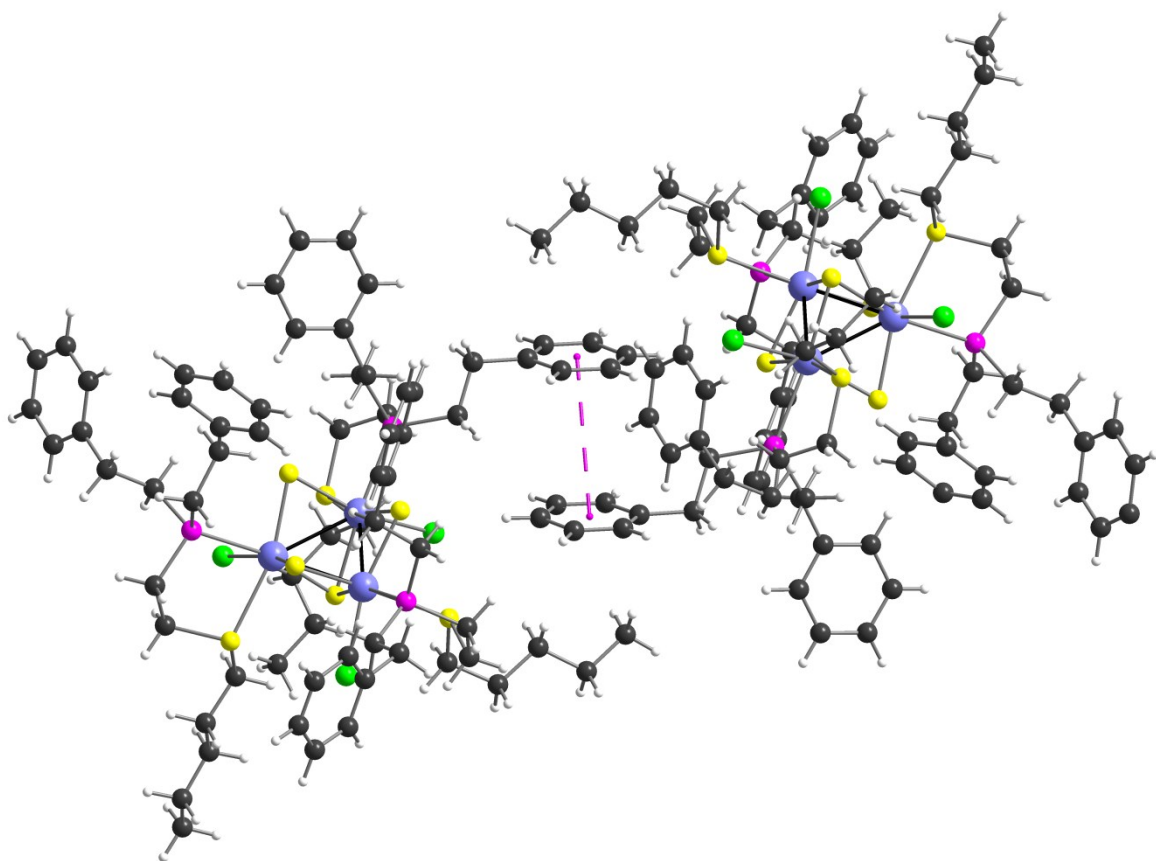


Figure S1. Intermolecular π - π interactions between Ph rings in the crystal structure of [2]PF₆·0.6CH₃CN

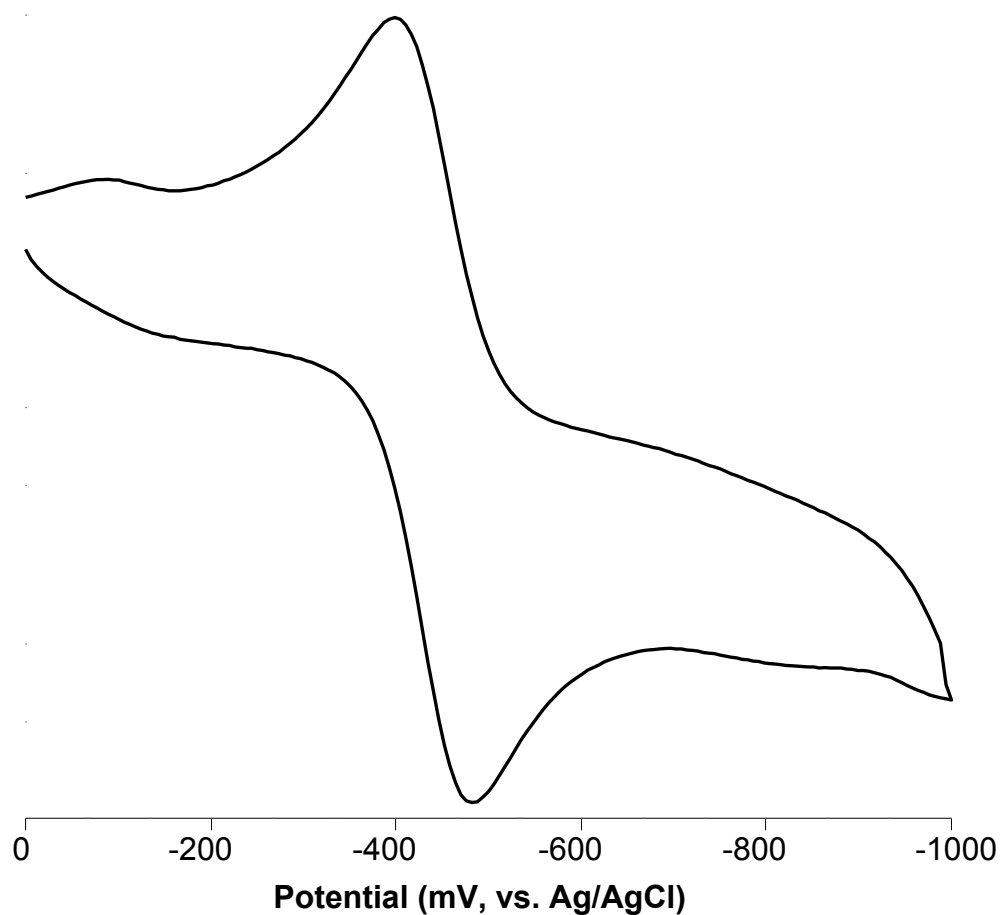


Figure S2. CV of [1]PF₆ in CH₃CN in the range from 0 to -1 V at scan rate of 0.1 V/s

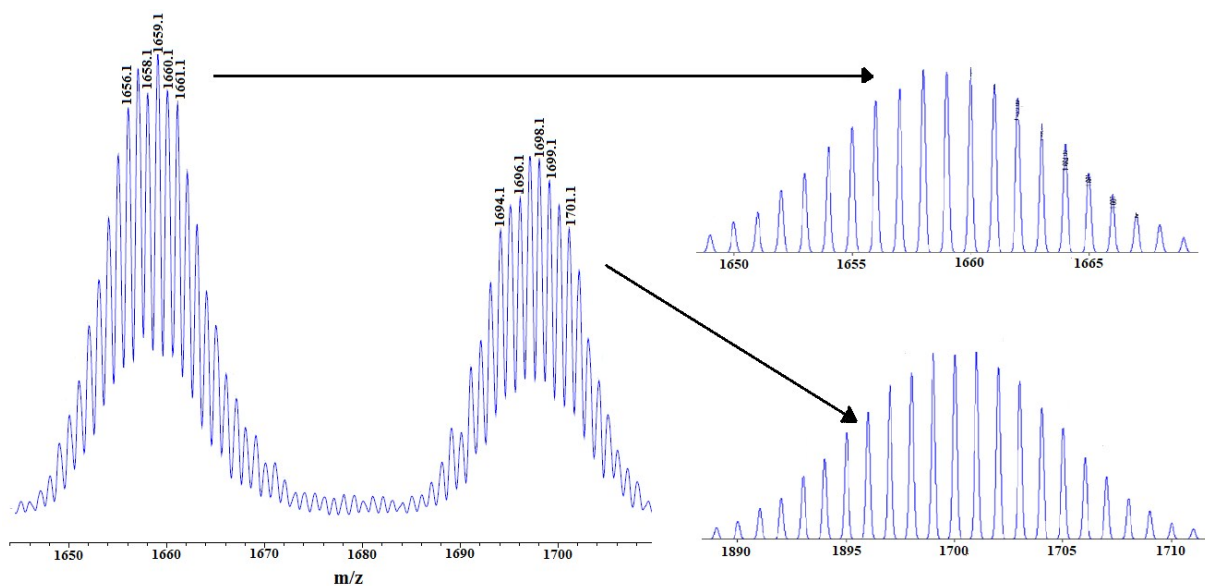


Figure S3. *Left:* ESI-MS of brown solution after filtration of green [1]PF₆. *Right:* Simulated isotopic distribution

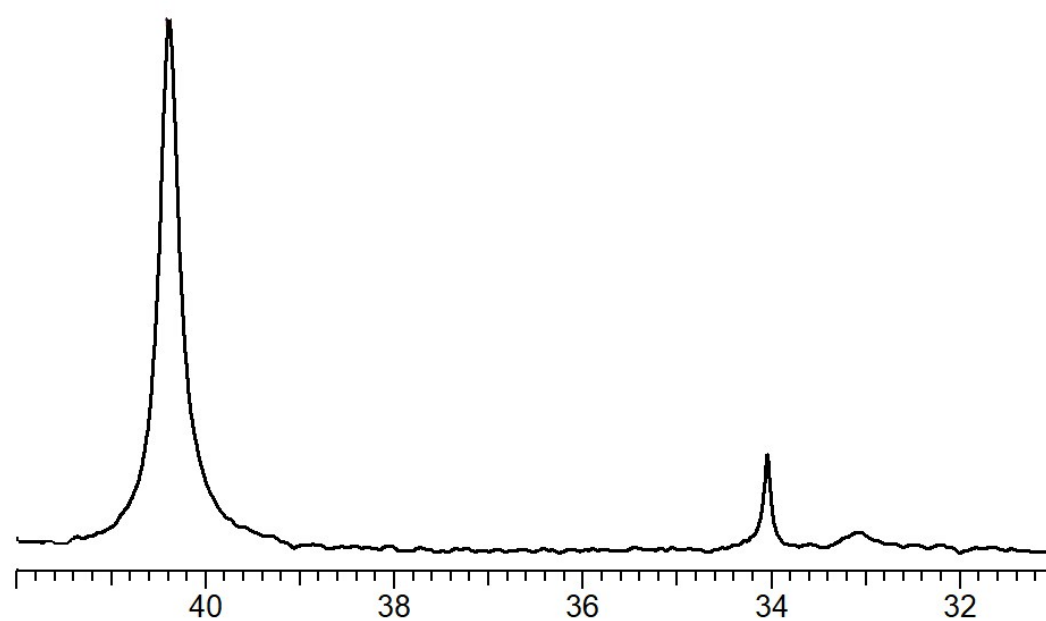
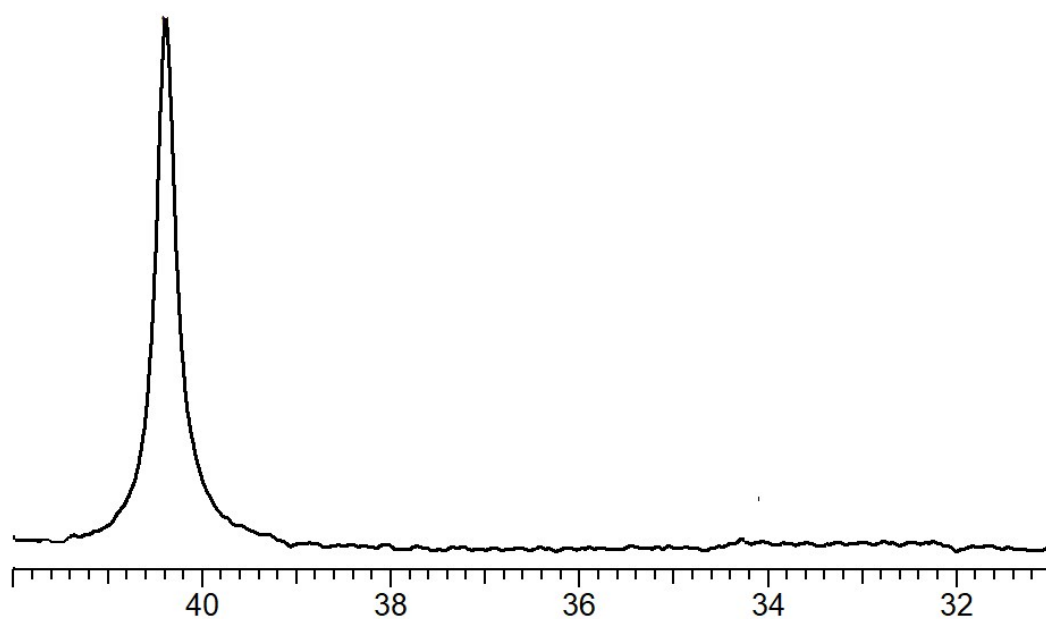


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectra of $[\mathbf{3}]\text{PF}_6^-$: before adding of Bu_4NCl (up); after three hours of reaction with Bu_4NCl (down)

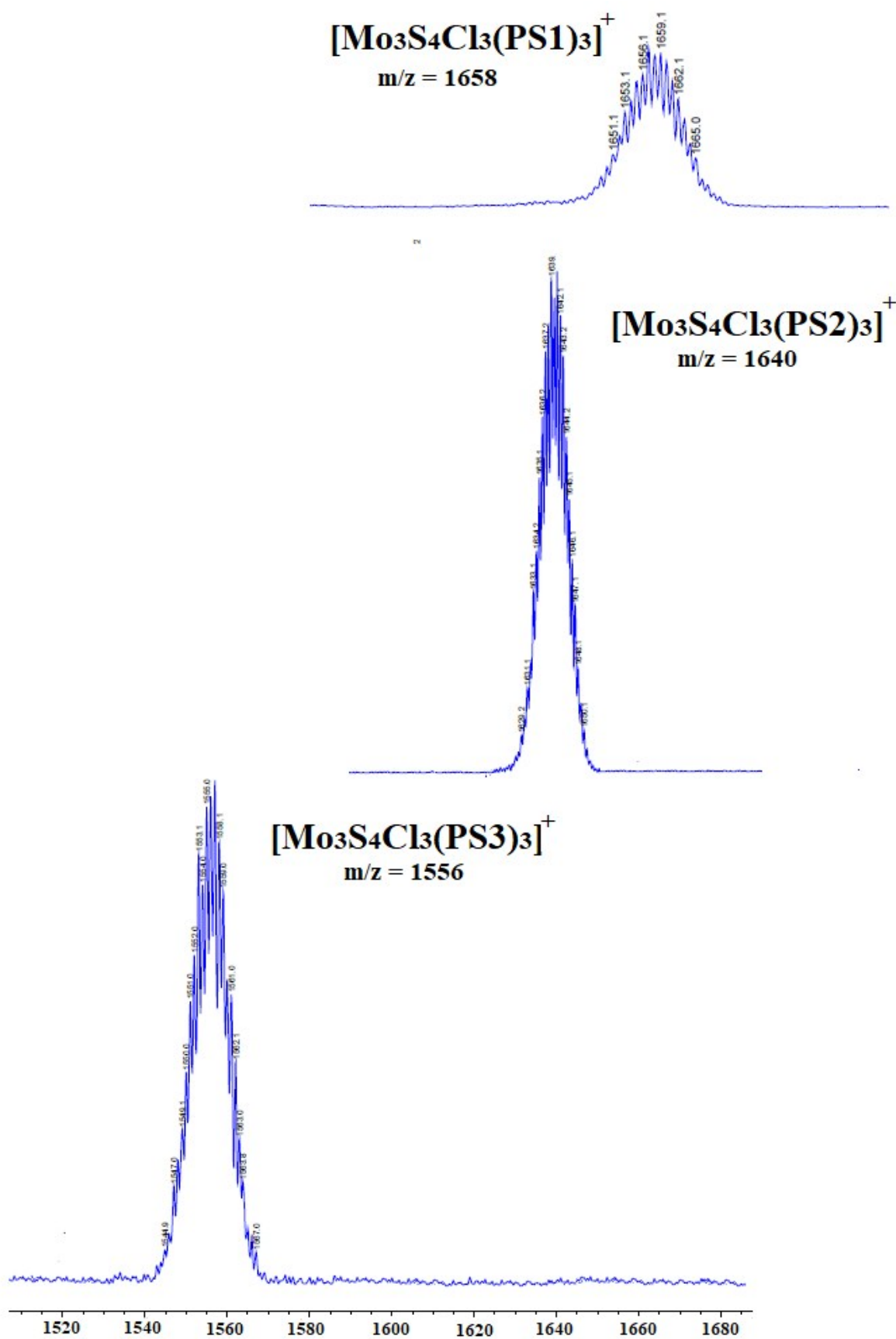


Figure S5. ESI-MS of $[\text{Mo}_3\text{S}_4\text{Cl}_3(\text{PS})_3]^+$ species after reactions of nitrobenzene reduction