Electronic Supplementary Information

Molybdenum based metallomicellar catalyst for controlled and selective sulfoxidation reactions in aqueous medium

R. D. Chakravarthy, V. Ramkumar and D. K. Chand

Department of Chemistry, Indian Institute of Technology Madras, Chennai, India.

E-mail: dillip@iitm.ac.in

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Figure S3: ORTEP diagram of the complex (C\textsubscript{19}H\textsubscript{42}N\textsubscript{2})\textsubscript{2}[MoO(O\textsubscript{2})\textsubscript{2}(C\textsubscript{2}O\textsubscript{4})]\cdot H\textsubscript{2}O with 50% thermal ellipsoids

Table S1: Crystallographic data and parameters for complex (C\textsubscript{19}H\textsubscript{42}N\textsubscript{2})\textsubscript{2}[MoO(O\textsubscript{2})\textsubscript{2}(C\textsubscript{2}O\textsubscript{4})]\cdot H\textsubscript{2}O

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**Figure S4:** Powder XRD pattern of the bulk complex $(C_{19}H_{42}N)_2[MoO(O_2)_{2}(C_2O_4)]\cdot H_2O$ compared with the simulated data.
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Determination of critical micelle concentration of \((C_{19}H_{42}N)_2[MoO(O_2)_{2}(C_2O_4)] \cdot H_2O\)

Electrical conductivity method was employed to determine the critical micelle concentration (CMC) of the complex \((C_{19}H_{42}N)_2[MoO(O_2)_{2}(C_2O_4)] \cdot H_2O\). The conductivity experiments were carried out in a double-jacket flask. The temperature of the flask was maintained at 25 °C by circulating water with Julabo FP50 Refrigerated - Heating Circulators. A SYSTRONICS digital bench top conductivity meter (Model 306) was used for the measurements. Solutions were prepared in deionised water which was first filtered with a Millipore Milli-Q system. A step-by-step dilution-extraction method was adopted for the measurements of specific conductance of the complex at various concentrations in order to avoid dilution error. The conductance was plotted as a function of molar concentration and the inflection point gives the value of CMC which is indicated in the figure S6.

**Procedure for the recyclability of the catalyst**

In a centrifuge tube, molybdenum complex (0.032g, 2.5 mol%) and thioanisole (0.186g, 1.5 mmol) in 2.5 ml of water were taken and stirred at room temperature. Then 40% (w/v) hydrogen peroxide (0.128ml, 1.5 mmol) was added slowly into the reaction mixture. Stirring was continued for 10 min. Reaction progress was monitored by TLC. After completion, ethyl acetate was added to it and the reaction mixture was centrifuged and decanted to separate molybdenum compound. The residual compound obtained was dried and used for second run. The aqueous phase is extracted with ethyl acetate 3-4 times. Then the combined organic extracts were dried over anhydrous sodium sulfate and the solvent was removed under reduced pressure. The crude product thus obtained was purified by column chromatography with Hexane: Ethyl acetate as an eluent.

For the second run: To the residual catalyst in the centrifuge tube, 2.5 ml of water and hydrogen peroxide (0.128ml, 1.5 mmol) was added. The mixture was stirred for 30 min to activate the catalyst. Then thioanisole (0.186g, 1.5 mmol) was added and stirring was continued for 45 min. Reaction progress was monitored by TLC. After completion, ethyl acetate was added to it and the reaction mixture was centrifuged and decanted to separate molybdenum compound. The residual compound was dried and used for the subsequent cycle.

After 4 run, 0.013g of catalyst was recovered. So in each run, on an average of 81 % catalysts can be recovered.