Electronic Supplementary Information

Deep oxidative desulfurization of dibenzothiophene with {Mo_{132}} nanoball supported on activated carbon as efficient catalyst at room temperature

Ali Mojaverian Kermani[a], Ali Ahmadpour[a,*], Tahereh Rohani Bastami[b], Mahboube Ghahramaninezhad[b]

[a] Department of Chemical Engineering, Faculty of Engineering, Ferdowsi University of Mashhad, Mashhad, Iran

[b] Department of Chemical Engineering, Quchan University of Technology, Quchan, Iran

*Corresponding author: Tel/fax: +98 51 38805006;
E-mail address: ahmadpour@um.ac.ir

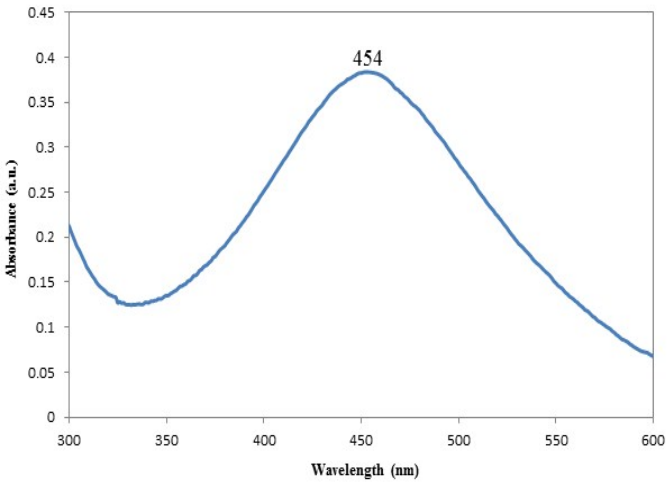


Fig. S1. UV-Vis spectrum of $\{Mo_{132}\}$ aqueous solution

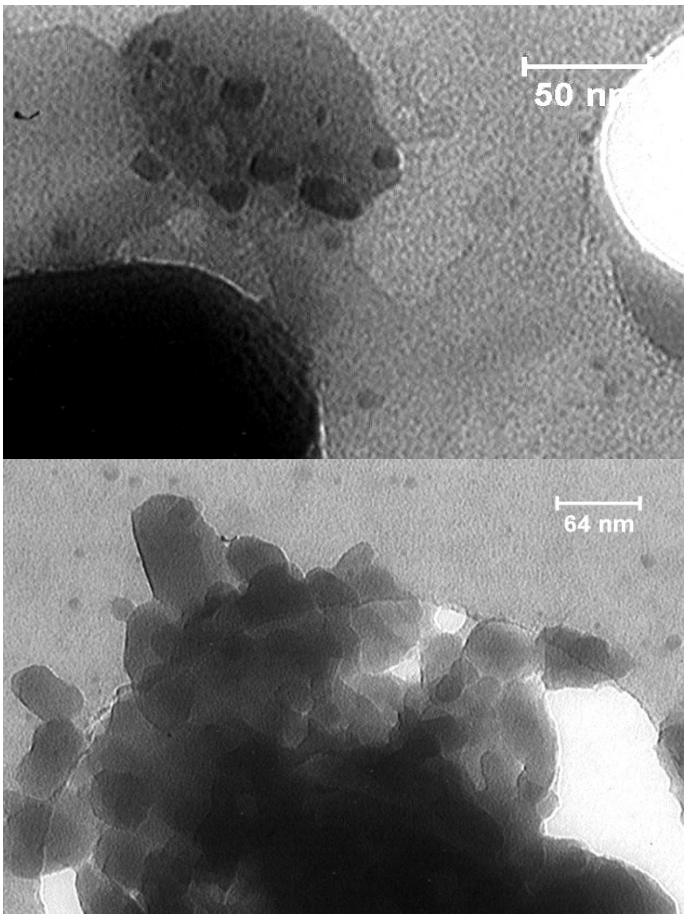


Fig. S2. TEM images of prepared $\{Mo_{132}\}$ in ethanol

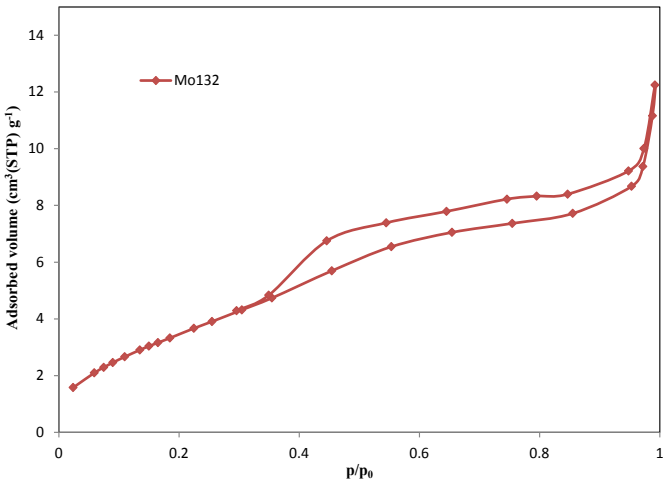


Fig. S3. Nitrogen adsorption/desorption isotherms of $\{Mo_{132}\}$

H_2-TPR analysis:

The H_2-temperature programmed reduction (H_2-TPR) experiment was performed on 50 mg of the catalyst ({Mo_{132}}/AC-20) placed in a U-shaped quartz reactor. Prior to the TPR run, the catalyst was degassed in flow of 10 sccm Ar at 110℃ for 1 hour, and cooled down to 40℃. Then, the sample was heated from 40 to 900℃ at a heating rate of 10℃/min in a flow of 5% H_2/Ar mixture (10 sccm).

The H_2-TPR was employed to study the reducibility of the catalyst. As shown in Fig. S4, {Mo_{132}}/AC-20 exhibited two reduction peaks, a sharp peak at 560^{o}C and a weak peak at higher temperature of 710 ^{o}C. These two peaks indicate reduction of Mo^{VI} and Mo^{VI} in {Mo_{132}} cluster in the catalyst.

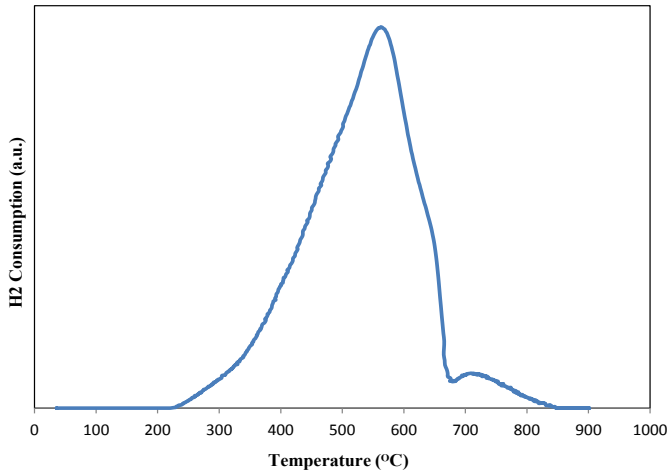
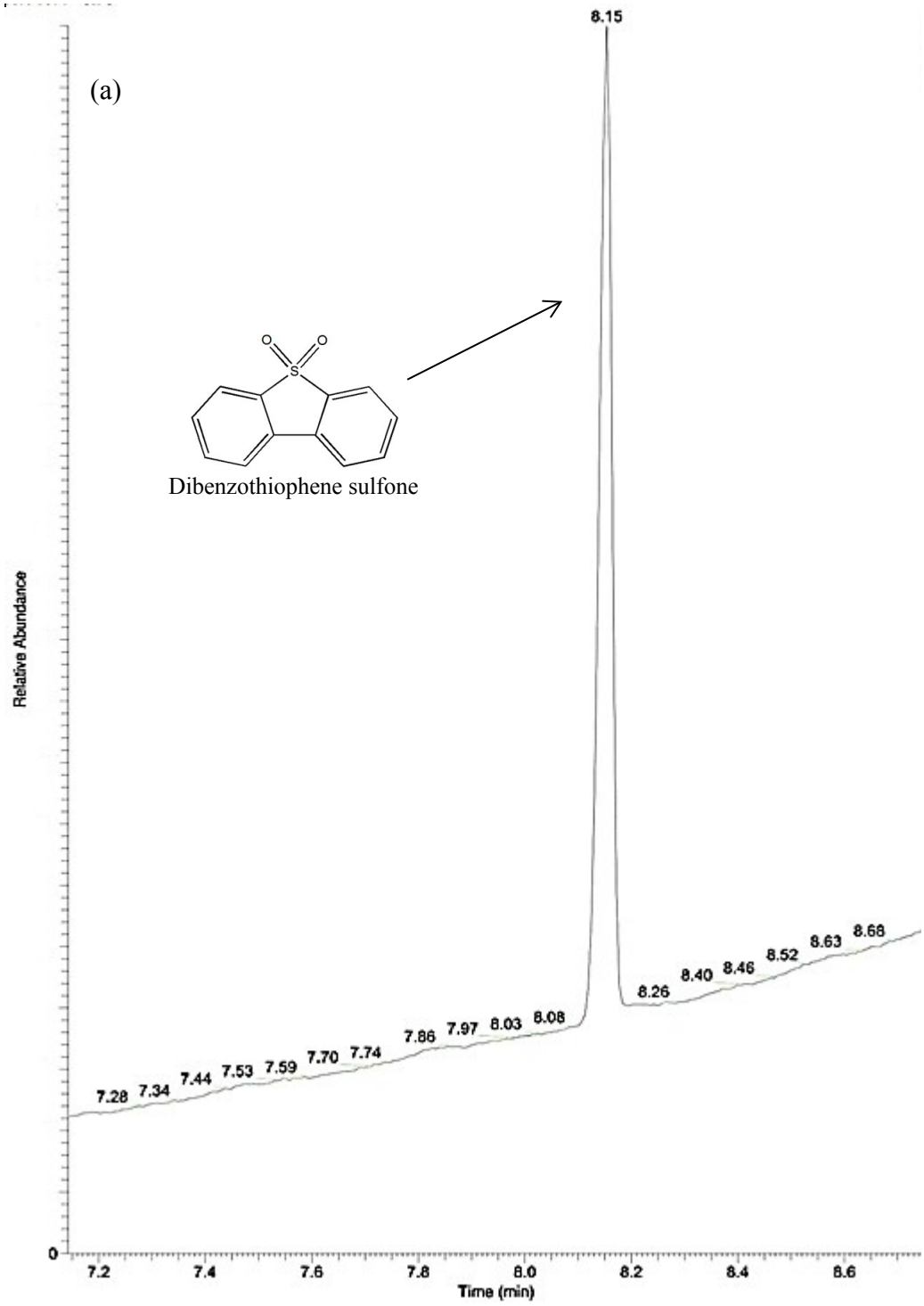


Fig. S4. H_2-TPR profile of {Mo_{132}}/AC-20

Table S1

Reusability of {Mo_{132}}/AC-20 and {Mo_{132}} content of the catalyst in each step

Catalyst samples	DBT removal (%)	Actual {Mo_{132}} contents (%)
Fresh catalyst	99.5	9.04
1st reuse	98.1	8.59
2nd reuse	97.8	8.38
3rd reuse	97.7	8.35


(a)
Dibenzothiophene sulfone
Relative Abundance
Time (min)
8.15
8.26
8.40
8.46
8.52
8.63
8.68
7.28
7.34
7.44
7.53
7.59
7.70
7.74
7.86
7.97
8.03
8.08
0
7.2
7.4
7.6
7.8
8.0
8.2
8.4
8.6

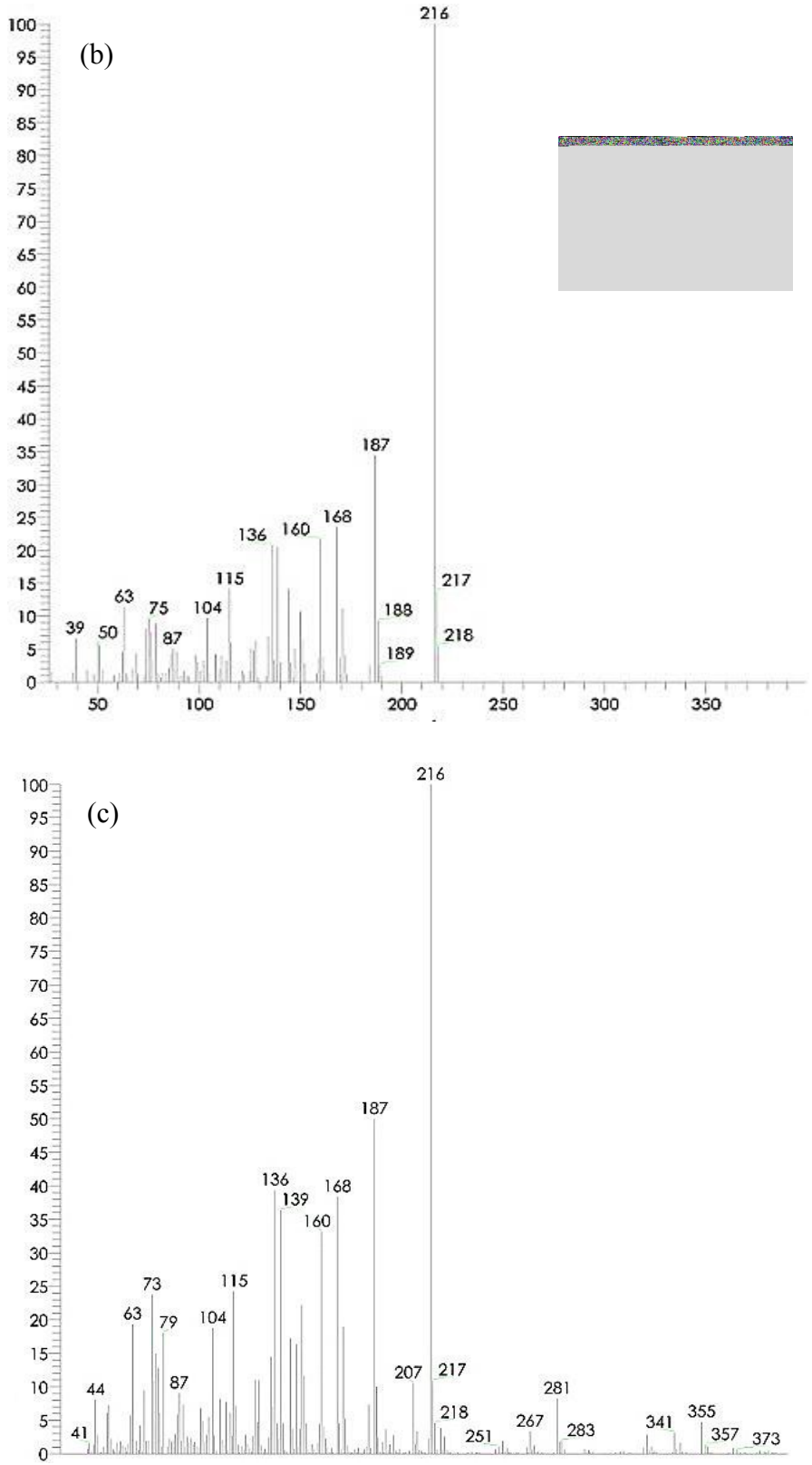


Fig. S5. GC-MS analysis of the acetonitrile phase at the end of the process. (a) GC-MS chromatogram, (b) The standard mass spectrum of DBT sulfone, (c) The mass spectrum of the oxidation product of DBT. Reaction condition: T = 25 ^{o}C, {Mo_{132}}/AC-20 catalyst dosage = 0.0025 g cat/ g F, O/S = 10, t = 30 min, initial sulfur content = 500 ppm.