Selective Oxidation of Sulfides Catalysed by WO_3 Supported on Chitosan-Derived Carbon

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SUPPLEMENTARY INFORMATION

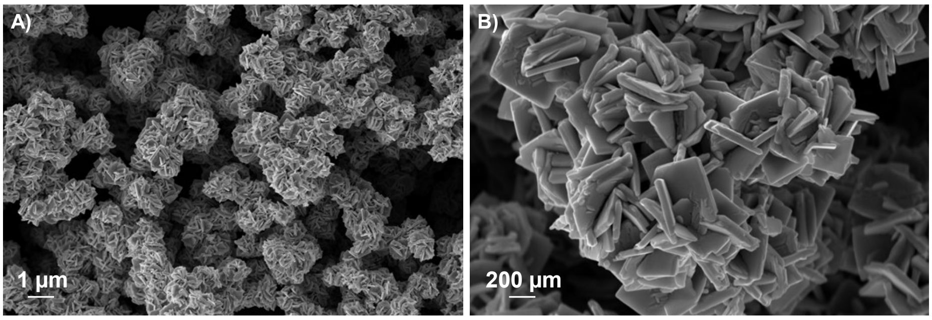

Figure S1. A-B) SEM images of the WO_3.

Table S1. Comparison of catalytic conditions with other previous works.

Catalyst	Solvent	Temperature (°C)	Time (h)	Substrate (mmol)	Oxidizer	Yield (%)	Product	Ref.
TaC	Methanol	45°C	1.25	1	H_2O_2	97	Sulfoxide	60
NbC	Ehanol	60°C	2.75	1	H_2O_2	98	Sulfone	60
SBTIC[a]	Dichloromethane/ Methanol	25°C	1.5	2	H_2O_2	82	Sulfoxide	62
C_6F_{14}	Dichloromethane	25°C	48	1	m-CPBA	87	Sulfone	63
$NiWO_4$/ chitosan	Acetonitrile	50°C	1	0,1	H_2O_2	>99	Sulfone	34
$Fe_2(MoO)_4$/ chitosan	Acetonitrile	50°C	0.5	0,1	H_2O_2	99	Sulfone	33
α-Ag_2WO_4:V	Acetonitrile	50°C	1	0,1	H_2O_2	>99	Sulfone	28
α-Ag_2WO_4	Acetonitrile	50°C	0.5	0,1	H_2O_2	>99	Sulfone	29
$WO_3 \cdot H_2O$	Octane	70°C	1	-	H_2O_2	>98	Sulfone	65
WO_3	Tetrahydrofuran	0°C	40	1	H_2O_2	90	Sulfoxide	66

[a]Silica-Based Tungstate Interphase Catalyst; [b] in the presence of cinchona alkaloids.

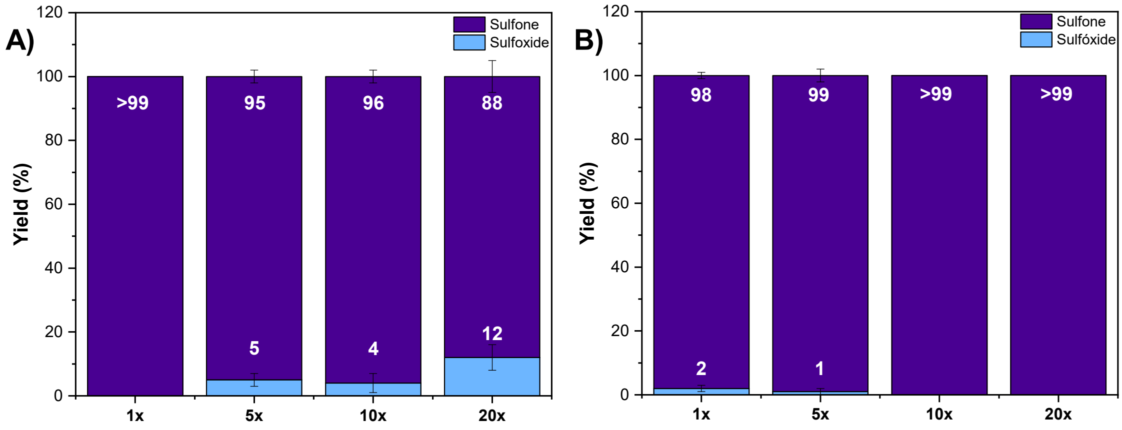

Figure S2. Scaling using **A)** acetonitrile and **B)** water as a solvent reaction.

Catalytic Substrate Scope. The detection of sulfides and their corresponding sulfones was performed under specific chromatographic conditions for each compound. For thioanisole/methyl phenyl sulfone (CAS 100-68-5, rt = 2.2 min; CAS 3112-85-4, rt = 3.9 min), 4-methoxythioanisole/4-methoxyphenyl methyl sulfone (CAS 3517-90-6, rt = 5.2 min; CAS 3517-90-6, rt = 5.0 min), 4-methyl p-tolyl sulfide/4-(methylsulfonyl)toluene (CAS 623-13-2, rt = 2.7 min; CAS 31855-99-7, rt = 4.5 min), 4-nitrothioanisole/1-(methylsulfonyl)-4-nitrobenzene (CAS 701-57-5, rt = 3.9 min; CAS 2976-30-9, rt = 4.8 min), diethyl sulfide/diethyl sulfone (CAS 352-93-2, rt = 1.7 min; CAS 597-35-3, rt = 2.1 min), 4-chlorothioanisole/4-chlorophenyl methyl sulfone (CAS 123-09-1, rt = 3.1 min; CAS 98-57-7, rt = 4.6 min), 2,5-dimethylthiophene/2,5-dimethylthiophene sulfone (CAS 638-02-8, rt = 1.2 min; CAS 50590-75-9, rt = 4.1 min), and dibenzothiophene/dibenzothiophene sulfone (CAS 132-65-0, rt = 5.3 min; CAS 1016-05-3, rt = 6.2 min), the oven temperature was initially set to 75°C for 2 minutes, followed by a ramp of 20°C/min to a final temperature of 325°C, held for 2 minutes. For thiophene/thiophene 1,1-dioxide (CAS 110-02-1, rt = 1.7 min; CAS 2976-30-9, rt = 1.5 min), the temperature ramp was adjusted to 5°C/min from 75°C to 325°C, with an initial hold of 2 minutes and a final hold of 2 minutes. Similarly, diphenyl sulfide/diphenyl sulfone (CAS 139-66-2, rt = 21.8 s; CAS 127-39-9, rt = 5.7 min) was analyzed with an initial oven temperature of 40°C, held for 2 minutes, and ramped at 5°C/min to 325°C, held for 2 minutes. The method parameters included an inlet temperature of 325°C, a 1 μL injection volume in split mode, and nitrogen as the carrier gas. Data acquisition and analysis were carried out using Agilent OpenLab 3.5 software.