Electronic Supporting Information(ESI)

for

$Ti(Phen)(OC_2H_5)_2Cl_2$: a highly efficient catalyst for selective oxidation of organic sulfides to sulfoxides by hydrogen peroxide

Rong-Hui Wu, [a,b] Jing Wu，[a] Ming-XinYu [a] and Long-Guan Zhu *[a]

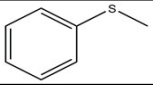
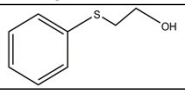
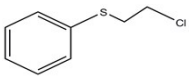
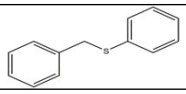
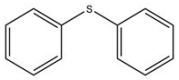
[a] *Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China.*

[b] *Key Laboratory of Chemical Utilization of Forestry Biomass of Zhejiang Province, Zhejiang A & F University, Lin'an, Zhejiang Province,311300,China.*

* To whom correspondene should be addressed

E-mail:chezlg@zju.edu.cn(L. G. Zhu).

Table S1 $Ti(Phen)(OC_2H_5)_2Cl_2$ catalyzed oxidation of organic sulfides with H_2O_2 in CH_3OH or CH_3CH_2OH solvent [a]

Entry	Substrate	Time (min)	CH_3OH	CH_3CH_2OH
			Conv. (%)/Sele. (%)[b, c]	Conv. (%)/Sele. (%)[b, c]
1		20	100 / 96	100 / 95
2		50	96 / 99	100 / 94
3		65	99/ 97	99 / 92
4		45	98 / 96	100 / 90
5		360	98 / 92	99/ 82

[a] Reaction conditions: 1.00 mmol of sulfides, 1.00 mmol of 30% H_2O_2, $2.5*10^{-3}$mmol Ti catalyst, in CH_3OH or CH_3CH_2OH solution (5 mL) at 25°C. Products were quantified by GC analysis and characterized by GC-MS.

[b] The GC yields (%) are measured relative to the starting sulfide.

[c] Selectivity to sulfoxides, the byproduct was sulfone.

Table S2 Crystallographic data and refinement parameters for complex 1

	1
Empirical formula	$C_{16}H_{18}N_2O_2TiCl_2$
Mr	389.12
Crystal system	Triclinic
Space group	P -1
Size(mm^3)	0.42×0.32×0.26
habit/color	Block/Colorless
a(Å)	9.0551(7)
b(Å)	9.1409(7)
c(Å)	11.4606(8)
α(°)	105.286(7)
β(°)	90.508(6)
γ(°)	104.462(7)
V($Å^3$)	883.22(27)
Z	2
Dc(Mg·m-3)	1.463
μ(mm^{-1})	0.796
θ range	3.2-25.1
Unique reflections	3127
Observed reflections	1924
parameters	210
F(000)	399.9
T(K)	293(2)
R_1 wR_2[I>2σ(I]	0.059, 0.139
R_1 wR_2[alldata]	0.102, 0.174
GOF	1.048
Largest peak and hole(e· Å-3)	0.370, -0.260

Table S3 Selected bond lengths (Å) and angles (°) for complex 1

Lengths			
Ti1-O1	1.788(4)	Ti1-O2	1.761(3)
Ti1-N1	2.249(4)	Ti1-N2	2.251(4)
Ti1-Cl1	2.4009(13)	Ti1-Cl2	2.3519(13)
Angles			
O1-Ti1-O2	105.06(18)	O1-Ti1-N2	162.80(16)
O2-Ti1-N2	91.43(16)	O1-Ti1-N1	90.74(16)
O2-Ti1-N1	163.23(15)	N2-Ti1-N1	72.40(14)
O1-Ti1-Cl1	92.92(11)	O2-Ti1-Cl1	90.58(11)
N2-Ti1-Cl1	81.91(9)	N1-Ti1-Cl1	82.92(9)
O1-Ti1-Cl2	97.20(11)	O2-Ti1-Cl2	97.86(11)
N2-Ti1-Cl2	85.07(10)	N1-Ti1-Cl2	85.42(10)
Cl1-Ti1-Cl2	164.65(6)		

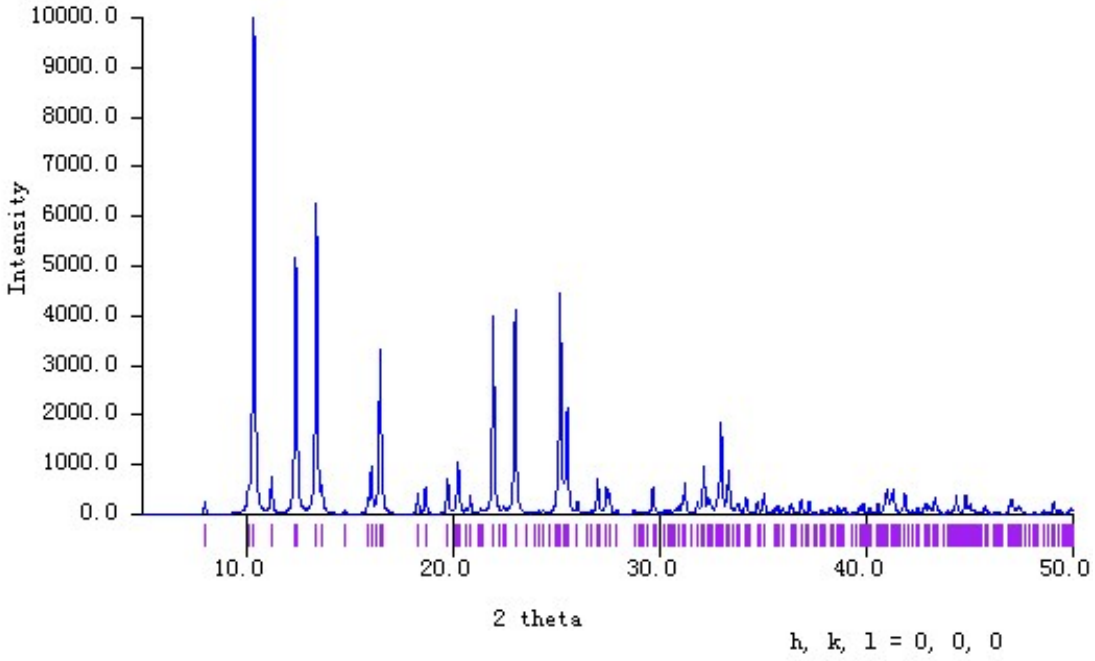


Figure S1. The calculated XRD pattern from single crystal data of complex 1.

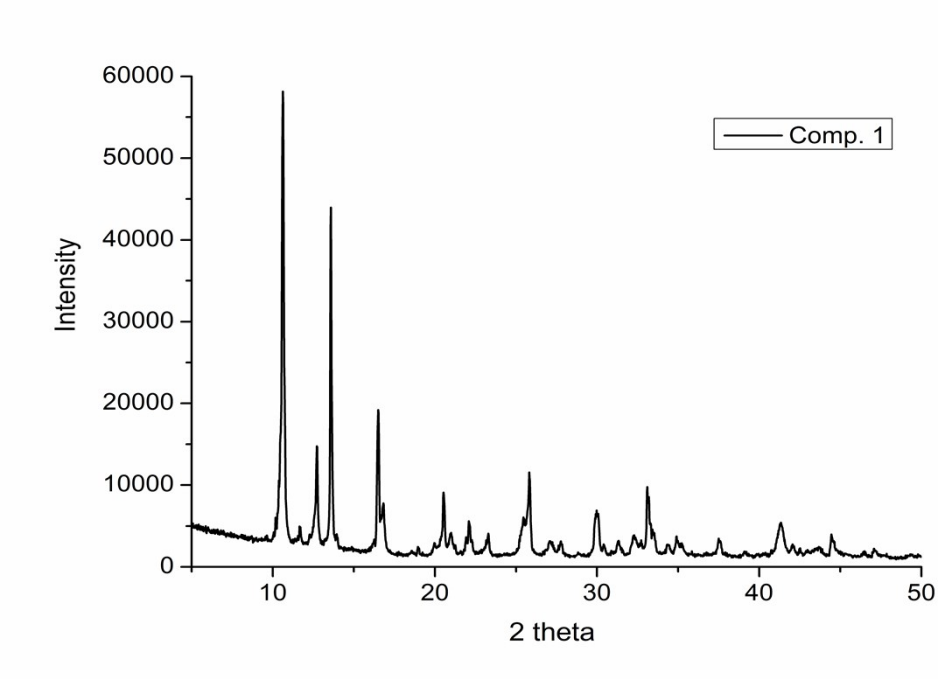


Figure S2. The powder XRD pattern for complex 1.

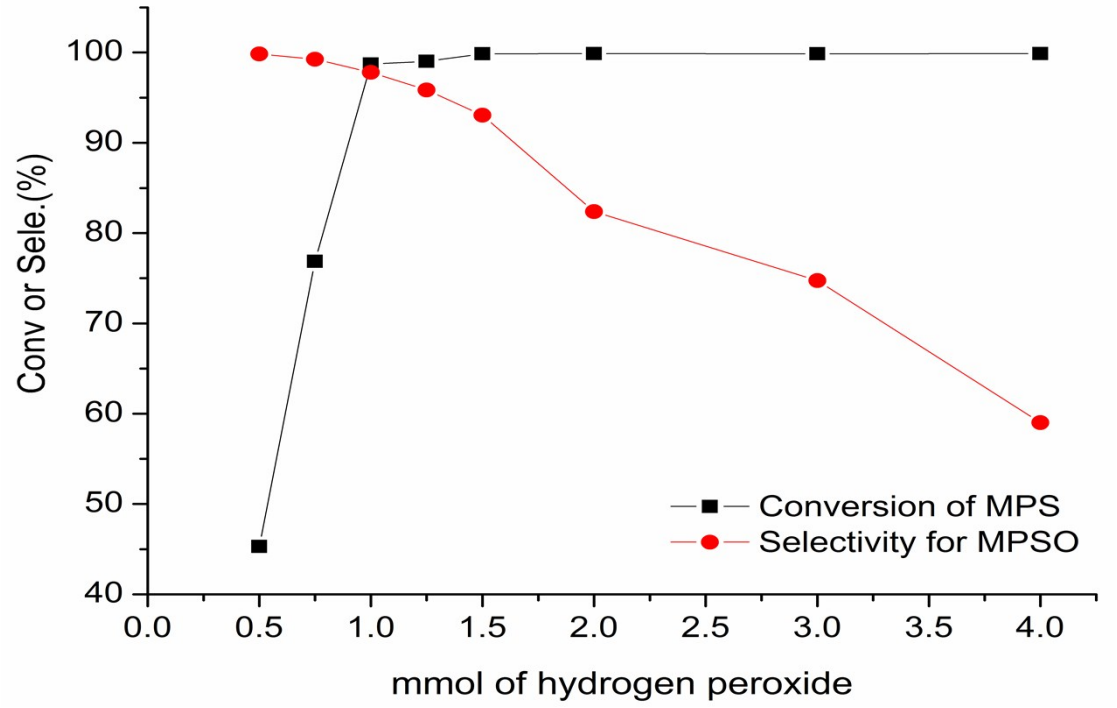


Figure S3. A hydrogen peroxide amount dependent profile of the oxidation of MPS by complex 1, the reactions were run for 20 min at 25 °C.

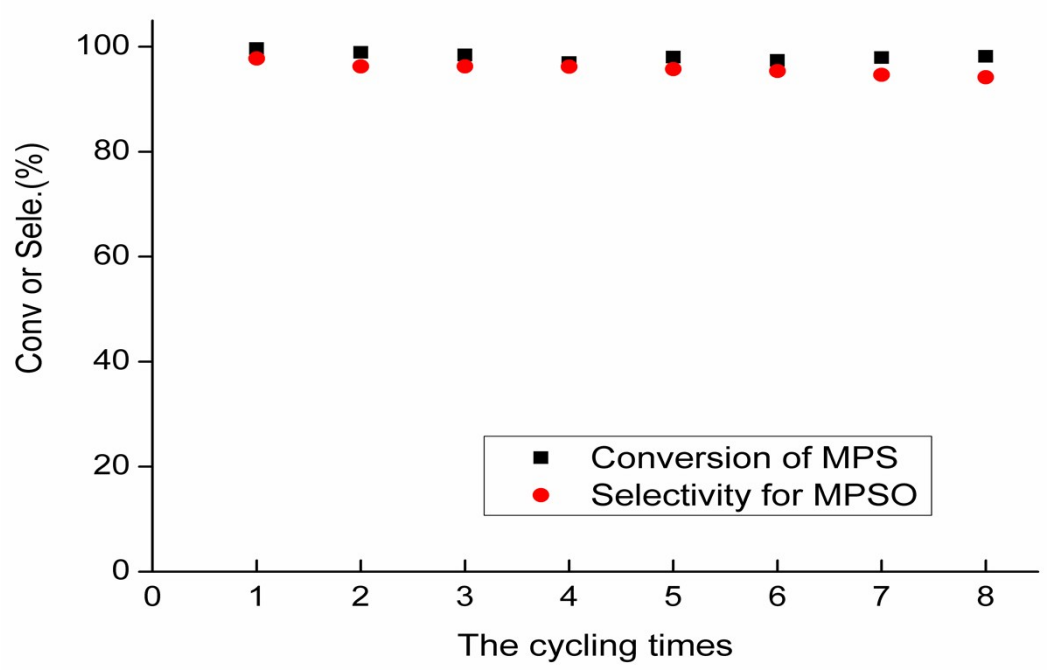


Figure S4. Catalytic activity of eight repetition cycles for complex 1

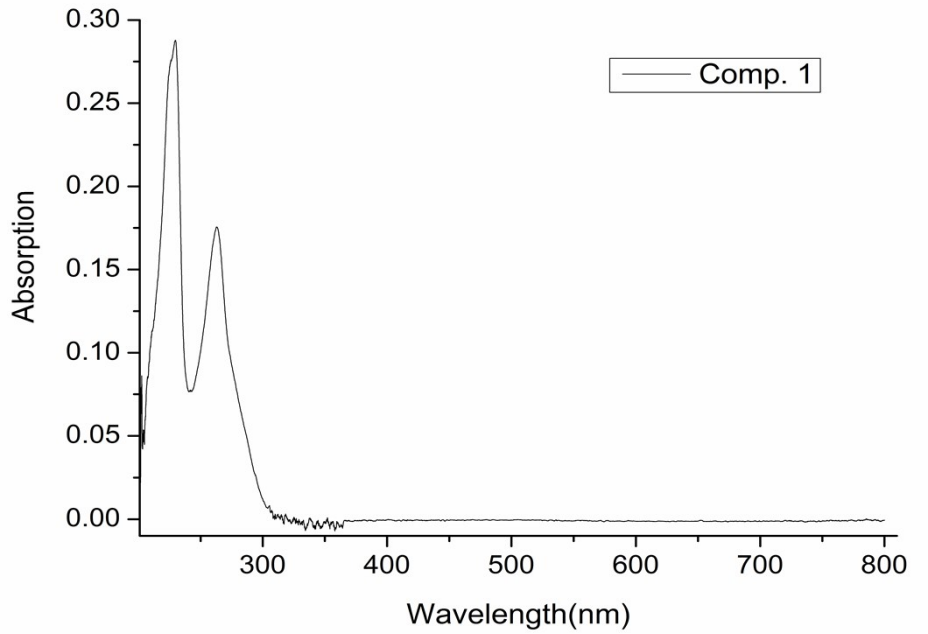


Figure S5. The UV-vis spectra of complex 1 in CH_3OH

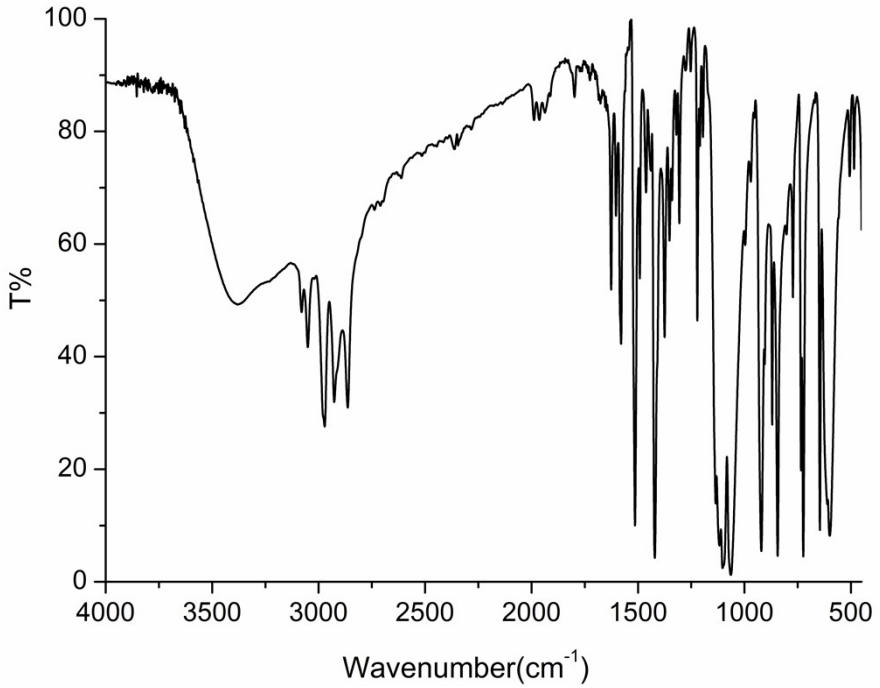


Figure S6. The IR spectrum of of complex 1.

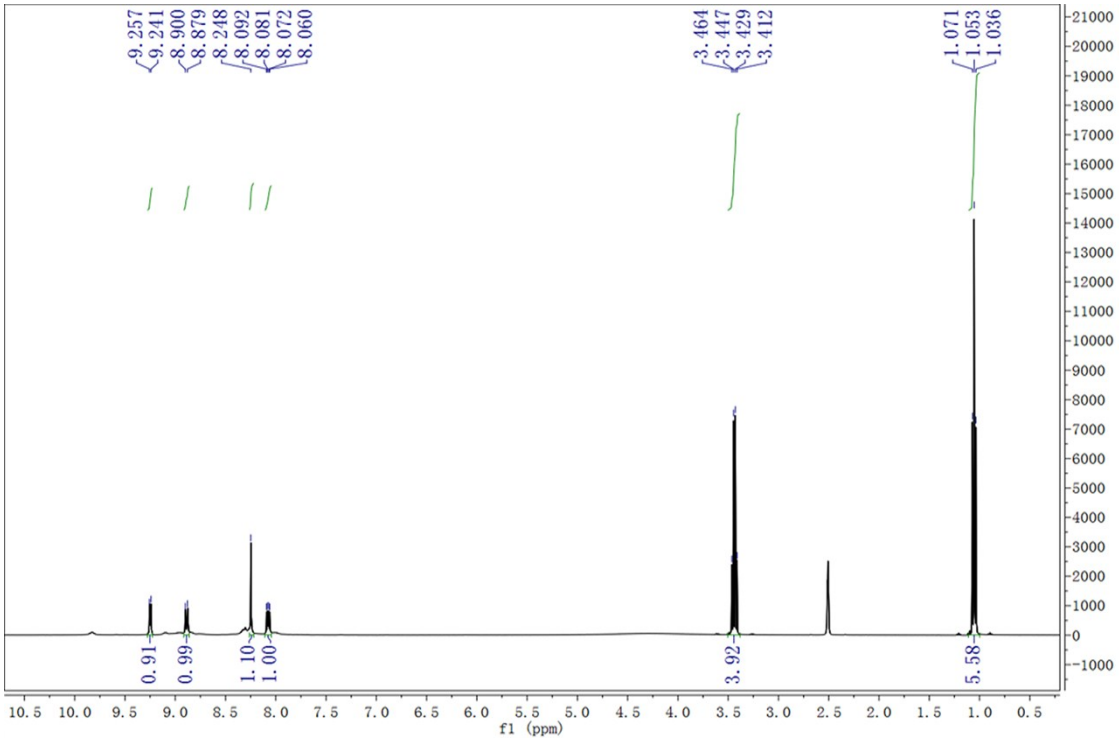


Figure S7. The ^{1}H NMR spectra of complex 1

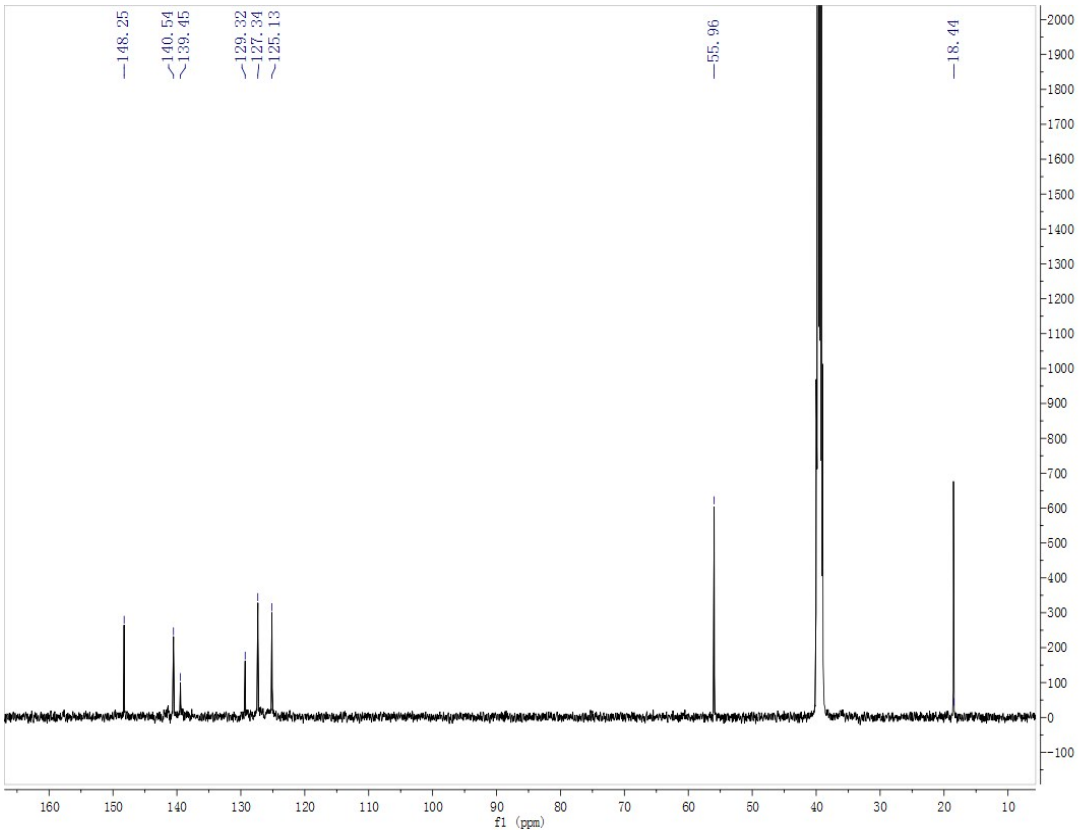


Figure S8. The ^{1}C NMR spectra of complex 1