TEMPO-mediated and co-reductive Effective and aerobic epoxidation of olefins using magnetically recoverable iron(III) bis(phenol) diamine complex

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Catalyst characterization



Figure S1: Magnetization curve of Fe₃O₄@SiO₂-APTES-FeL^{AE}.

Products analysis by GC

The reaction mixtures were analyzed by gas chromatography (GC, Agilent gas chromatograph model 7890A) equipped with an HP-1 methyl siloxane column (30 m in length _ 320 mm _ 0.25 mm) column with N₂ carrier gas and flame ionization detector (FID). The applied GC method to obtain a good separation of different compounds was: initial temperature 40 °C, initial time 4 min, temperature rise rate 10 °C/min, final temperature 250 °C and final time 5 min. To define the conversion of olefins and selectivity to epoxides, the certain concentration of anisole was used as internal standard. For instance, the typical GC spectra of alkenes epoxidation reaction, are demonstrated at Figure S6. The relative correction factor of epoxide to internal standard was determined using standard solution through following equation (Eq.1), where *f* was the relative correction factor, A_s was the peak area of internal standard, A_r was the peak area of alkene or epoxide in standard solution, C_s was the concentration of internal standard and C_r was the concentration of alkene or epoxide in standard solution.

$$f=(A_s/C_s)/(A_r/C_r)$$
(Eq.1)

The concentration of analyte (olefin, epoxide or TEMPO) after each catalytic reaction run was measured after the relative correction factor effect by Eq.2:

$$C_a = f \times A_a (A_s/C_s)$$
 (Eq.2)

 C_a was the concentration of analyte in solution after reaction completion, A_a was the peak area of analyte after reaction, A_s was the peak area of internal standard and C_s was the concentration of added internal standard to solution after reaction completion.

Accordingly, after defining the concentration of analyte after reaction finishing point, the conversion and selectivity was calculated by Eq.3 and Eq.4, respectively:

% Conversion=
$$\frac{moles \ of \ consumed \ alkene}{moles \ of \ alkene \ in \ the \ feed} \times 100$$
 (Eq.3)

% Selectivity to epoxide=
$$\frac{moles \ of \ produced \ epoxide}{moles \ of \ consumed \ alkene} \times 100$$
 (Eq.4)







Α







С



F



Ε







G





J





L



Κ







Μ



Ρ



0







Q



т



S







Figure S2. GC spectrum of sulfite-mediated and TEMPO-mediated alkene epoxidation reactions (A-V) under optimized conditions and internal standard (0.25 M).

U



Figure S3. Schematic representation of the calculated frontier molecular orbitals (FMOs) of the species involved in the proposed catalytic cycle in the presence of TEMPO in solution (water).



Figure S4. Schematic representation of the calculated FMOs of the species involved in the proposed catalytic cycle in the presence of SO_3^{2-} in solution (water).



Figure S5: Monitoring and hot filtration test of cyclopentene epoxidation reaction in the presence of A) Na₂SO₃ and B) TEMPO.





Figure S6: Recycling test of catalyst in epoxidation reaction of cyclopentene, in the presence of A) Na₂SO₃ and B) TEMPO.

Α



Figure S7: ¹H NMR of synthesized Bis(phenol) Diamine Ligand (H₂L^{AE})



Figure S8: FT-IR spectrum of Bis(phenol) Diamine Ligand (H_2L^{AE})



Figure S9: FT-IR spectrum of Bis(phenol) Diamine Ligand (H_2L^{AE-Br})