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Editorial

Catalytic Epoxidation Reaction

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1. Introduction

The epoxidation of unsaturated groups is a well-known process. There are different oxidizing agents (molecular oxygen, hydrogen peroxide, and percarboxylic acids), different phases (homogeneous vapor or liquid phase or liquid–liquid, gas–liquid–liquid, etc.), and essentially different substrates (from small gas molecules to triglycerides) (Contributions 1 and 2). Several studies have shown that producing epoxide compounds can present some risk because it is an exothermic process. Hence, one should design a suitable catalyst in an adequate reactor to work under safe operating conditions.

In this Special Issue, "Catalytic Epoxidation Reaction", we wish to showcase the diversity of this research area and focus on the research efforts in catalyst and process intensification. The topics include but are not limited to the following:

- The epoxidation of gaseous molecules;
- The epoxidation of molecules in multiphase;
- The epoxidation of triglycerides;
- Enzymatic catalysis;
- Catalyst preparation and characterization
- The benefits of process intensification for epoxidation reaction;
- Kinetic modeling.

Within the present Special Issue, eleven papers were collected, including nine research articles and two reviews. Both reviews comprehensively focus on all of the essential aspects needed for catalysis and process development (Contributions 1 and 2).

The research papers could be framed within different macro areas whose distribution is reported in Figure 1.

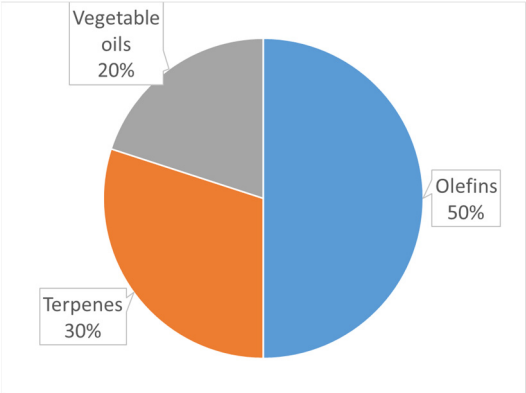

Figure 1. The distribution of papers per macro area of the Special Issue titled "Catalytic Epoxidation Reaction".

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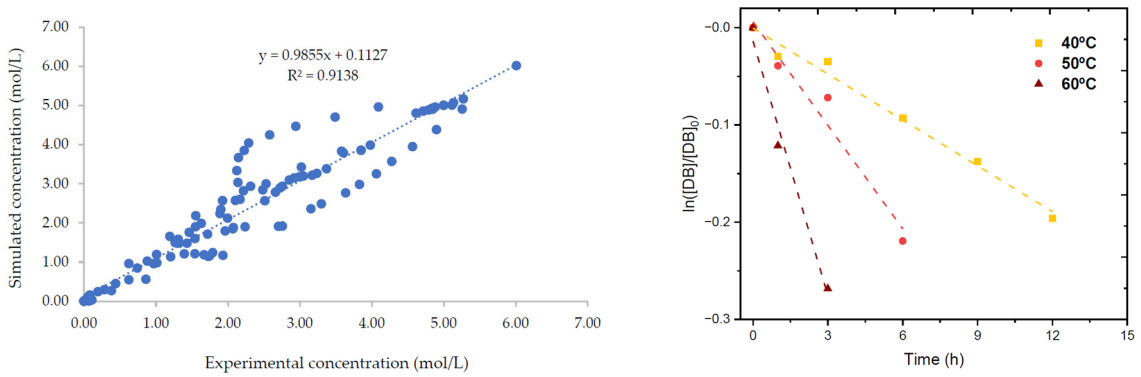
As revealed, the distribution is well balanced along three different macro areas, namely the epoxidation of (i) terpenes, (ii) vegetable oils, and (iii) olefins.

Moreover, 67% of the published papers were in the field of catalysis (i.e., the synthesis, characterization, and testing of heterogeneous catalysts), and the rest were in the field of chemical kinetics.

In the following sections, the main contributions of the SI will be reviewed and summarized, highlighting the point of novelty per each macro area.

2. Epoxidation of Vegetable Oils

Two articles on the epoxidation of vegetable oils were published within the present Special Issue. Meng et al. (Contribution 3) published an in-depth kinetic model for the epoxidation of cottonseed oil using perpropionic acid over Amberlite IR-120. The authors investigated a wide range of operation conditions, finding general rate expressions that were useful to interpret the data (see example reported in Figure 2A). The data had a good fit in every case, and the kinetic parameters were reliable.



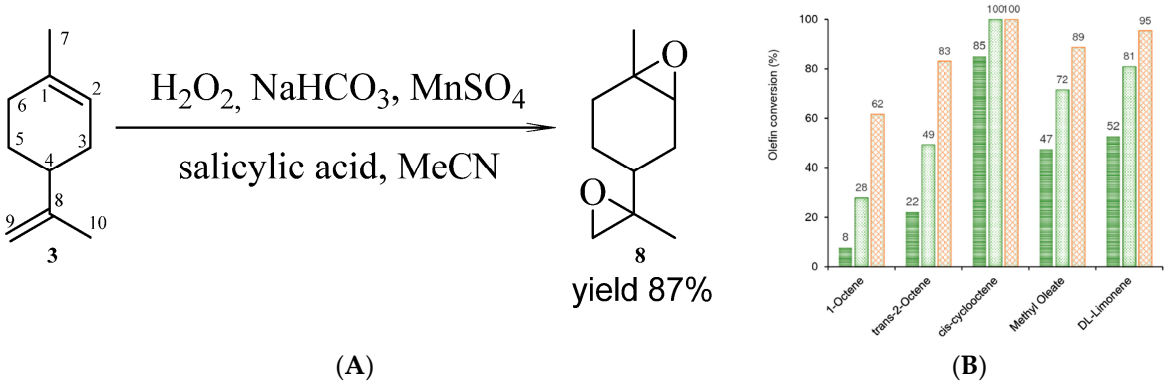
(**A**) (**B**)

Figure 2. (**A**) Parity plot of kinetic data reported in (Contribution 3). (**B**) First-order plot applied to experiments conducted at different temperatures (Contribution 4).

Catalá et al. (Contribution 4) epoxidized grapeseed oil in supercritical CO_2 using the Prileschajew method, demonstrating the advantages of working with supercritical carbon dioxide compared to conventional methods. The authors conducted a thorough kinetic investigation using simple modeling approaches, confirming the information reported in the literature regarding the reaction order (Figure 2B).

3. Epoxidation of Terpenes

Two published research papers focused on the epoxidation of terpenes. Fomenko et al. (Contribution 5) catalytically epoxidized 3-carene and limonene towards α-pinene epoxide, an important intermediate for fragrances, using hydrogen peroxide as an active oxidant with a new catalytic system. The authors proposed several synthetic strategies to increase the selectivity of the epoxide compounds by investigating the effects of solvent and reaction conditions. The catalytic system was utilized to produce a diepoxide by using limonene as a starting reagent (see Figure 3A). Gomes et al. (Contribution 6) used modified zeolites to epoxidize limonene and methyl oleate and identified active and selective materials for the tested reactions, i.e., Mo-TUD-type BEA zeolites (see Figure 3B).

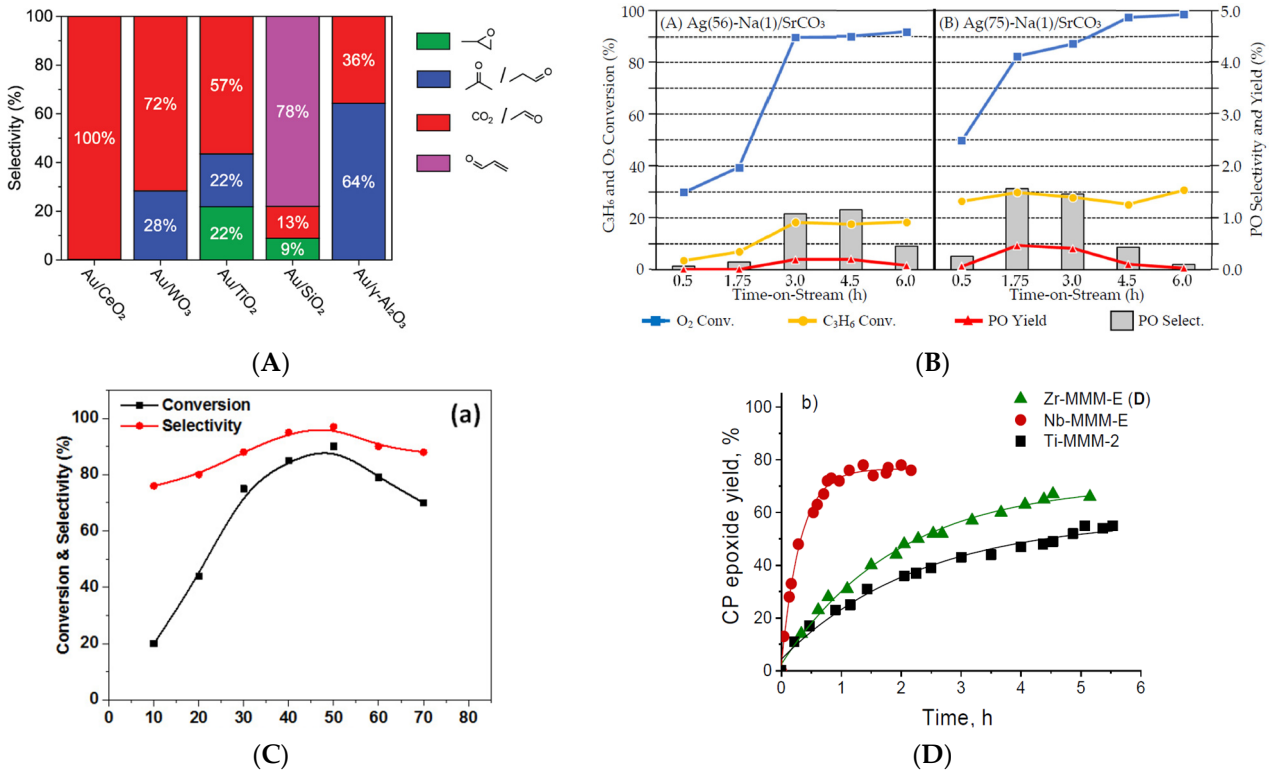


(**A**) (**B**)

Figure 3. (**A**) Preparation of limonene diepoxide (8) by epoxidation of limonene-3 (Fomenko et al., 2021) (Contribution 5). (**B**) Conversion of different substrates using Mo-TUD (IWI-acac) (TBHP, 70 °C) (Contribution 6).

4. Epoxidation of Olefins

Five published papers focused on the epoxidation of olefins. De Boed et al. (Contribution 7) proposed using gold-based catalysts for propene epoxidation, focusing on the effect of support on the reaction selectivity (see Figure 4A). The authors detected that the support had a strong influence on product selectivity in certain instances.



(**A**) (**B**)

(**C**) (**D**)

Figure 4. (**A**) Selectivity during the oxidation of propene at 200 °C in the presence of hydrogen over supported gold catalysts (Contribution 7). (**B**) Catalytic activity on Ag(56)-Na(1)/$SrCO_3$ and Ag(75)-Na(1)/$SrCO_3$ (Contribution 8). (**C**) Optimum reaction conditions for cyclohexene epoxidation using 10% Ni@CSs composites (Contribution 9). (**D**) *trans*-caryophyllene yield using different catalysts (Contribution 10).

Sugiyama et al. (Contribution 8) studied the same reaction using silver plasmon excitation technology with modified silver catalysts. The approach was indeed novel, and

while there were high olefin conversion rates, the selectivity towards propene oxide was not as pronounced (see Figure 4B).

Cyclohexene epoxidation was investigated by Alhumaimess (Contribution 9) by employing Ni-based heterogeneous catalysts. The study investigated the main reaction conditions' impact on the conversion and selectivity of the reaction, and it was found that Ni@CSs is a very active and selective catalyst (see Figure 4C).

Ivanchikova et al. prepared mesoporous zirconium silicates using two different methods: evaporation-induced self-assembly and the solventless organometallic precursor dry impregnation of commercial SiO_2. The catalysts demonstrated good activity and selectivity towards *trans*-caryophyllene epoxidation (see Figure 4D).

Finally, Freindorf and Kraka (Contribution 11) studied allylic alcohol Sharpless epoxidation via a quantum mechanical analysis, helping the scientific audience understand how molecules react and interact with the catalyst (see Figure 5). Their findings enable significant advancements in the computational-driven exploration of catalytic systems by integrating URVA with LMA, offering a powerful mechanistic approach for optimization.

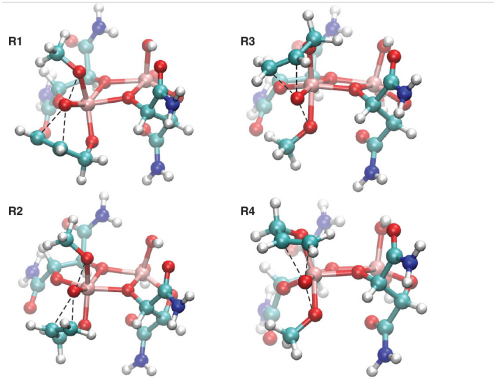


Figure 5. Transition state structures of catalyzed epoxidation reactions between methyl–hydroperoxide and allylalcohol (R1–R4), as studied by Freindorf and Kraka (Contribution 11).

5. Conclusions

This Special Issue can be considered successful as it demonstrates how epoxides of different nature can be obtained. The high quality of the collected papers, together with the highly interdisciplinary approach used, allowed for relevant papers to be produced in the sector, which will surely be references for future research.

Author Contributions: Conceptualization, all authors; writing—review and editing, all authors. All authors have read and agreed to the published version of the manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

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