

GREENER EPOXIDATION

「綠」光「環」 An important reaction in a water-organic solvent system

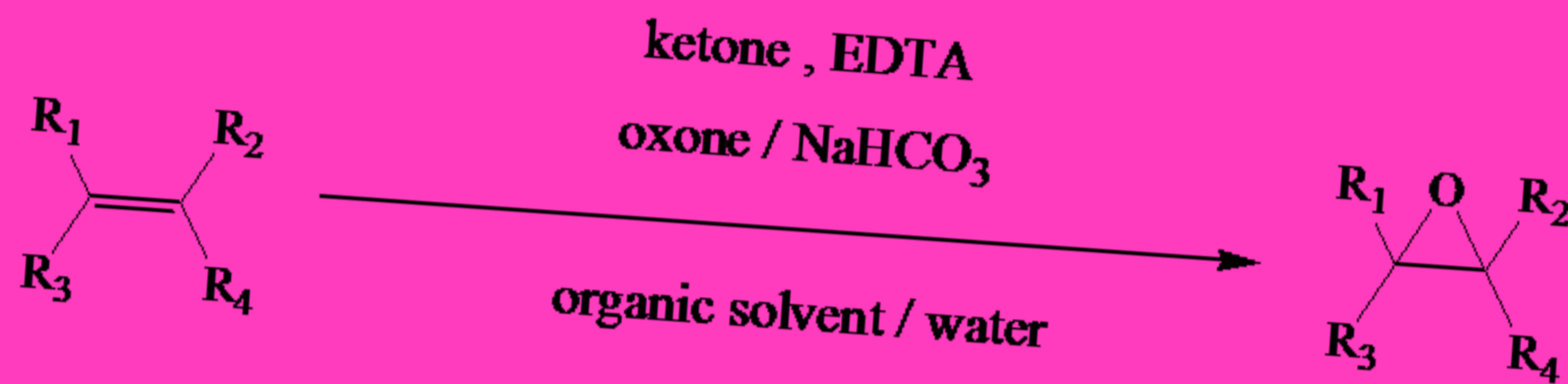
Introduction

In recent decades, experiments or production of materials in two-phase systems have become more popular. We would like to investigate the critical aspects in a suitable two-phase system.

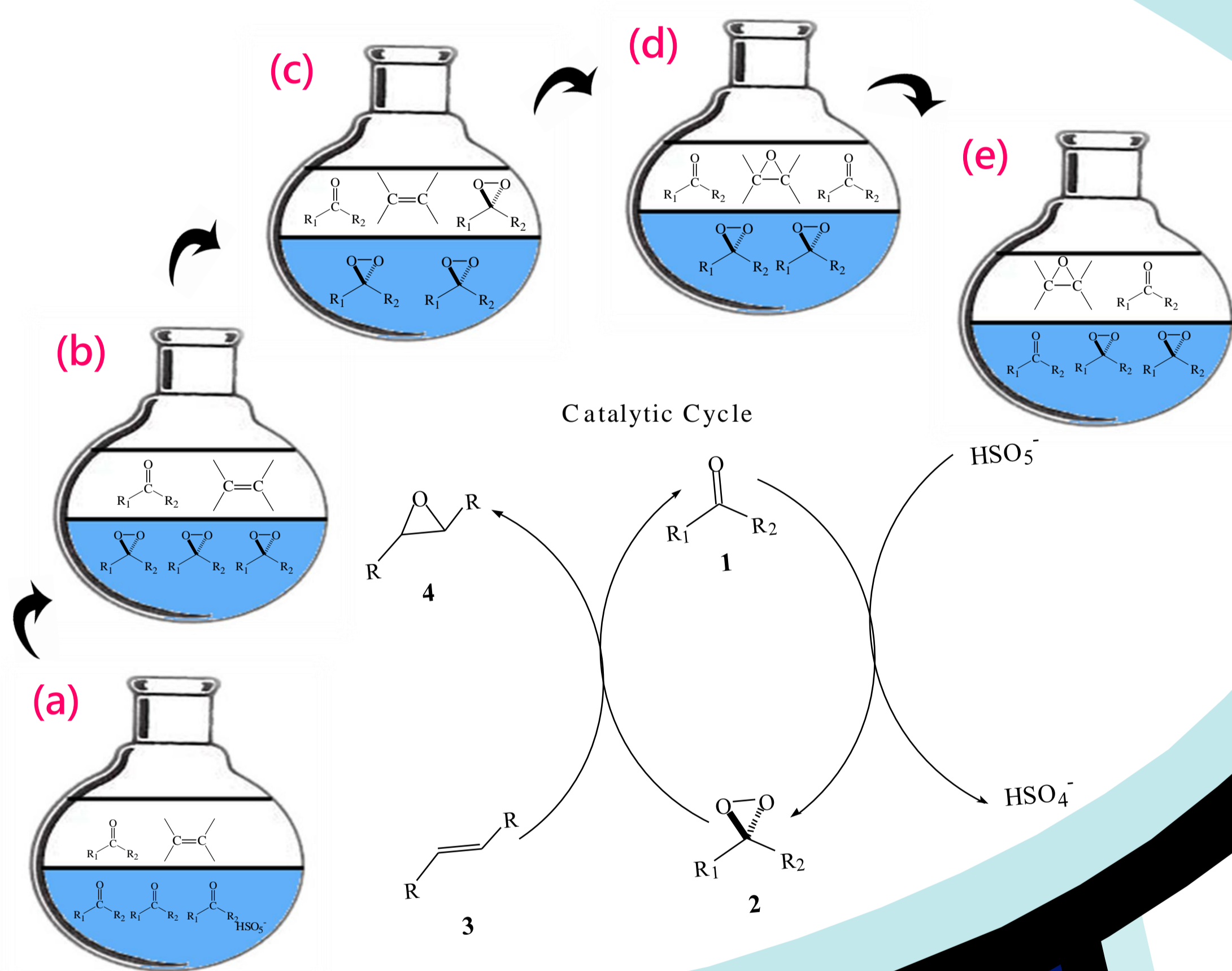
Why did we choose DIOXIRANE EPOXIDATION?

- potentially green - water is used as a solvent
- oxone is relatively a clean oxidizing agent
- paramount importance - it synthesizes drug precursors
- paradoxical results - conditions of epoxidation adopted not the same
- contradictory conditions adopted

In response to this, we try to put forward a generalized condition for two-phase dioxirane epoxidation through comprehensive investigations on ten different areas.

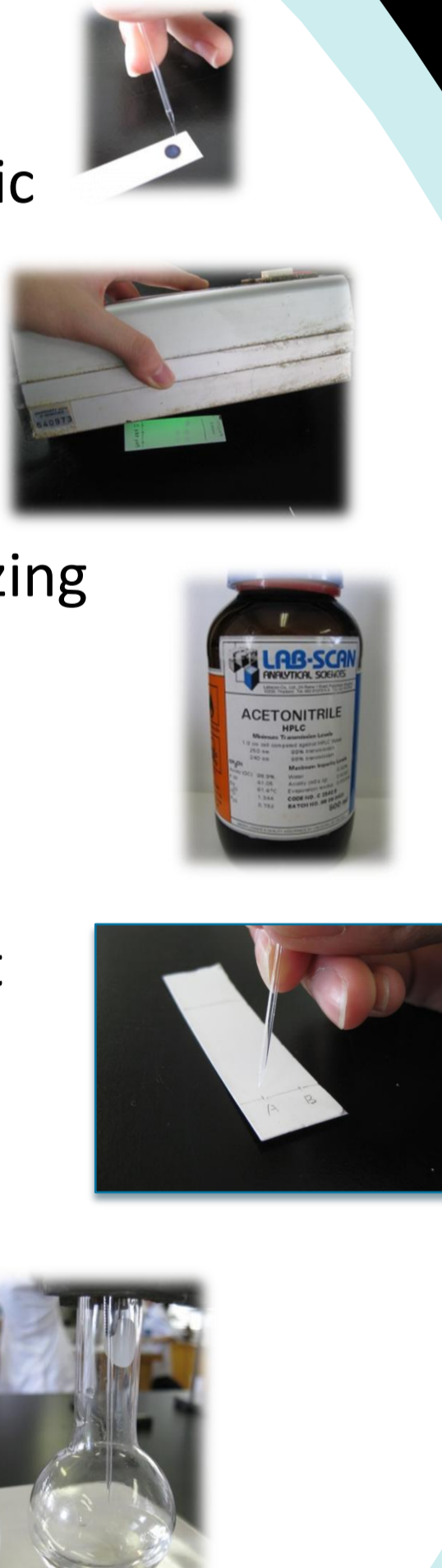


Mechanism of dioxirane epoxidation



The 10 areas of investigation of a greener epoxidation reaction

- 1) The best polarity of organic solvent compared to water
- 2) The most suitable catalyst
- 3) The most suitable water organic solvent ratio
- 4) Role of EDTA
- 5) The optimum temperature
- 6) The most suitable substrate to oxidizing agent ratio
- 7) The optimum substrate to catalyst ratio
- 8) The optimum pH value of water
- 9) The best substrate to catalyst ratio in respect to pH value
- 10) Alternative oxidizing agent



Conclusion

The general method for dioxirane epoxidation is under the mechanism of

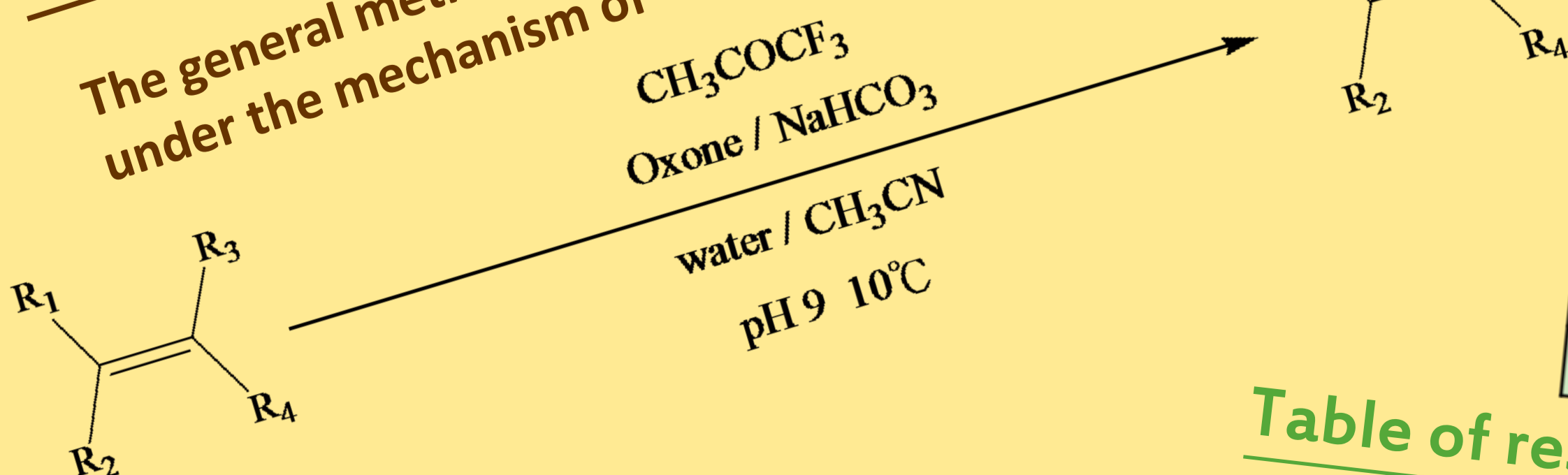


Table of results

The most suitable and "greener" system for two-phase dioxirane epoxidation	
1. Organic solvent	Acetonitrile
2. Additives in water	EDTA not needed
3. Catalyst	1,1,1-trifluoroacetone
4. Water to organic solvent ratio	1 : 1.1
5. Temperature	10°C
6. Substrate to oxone ratio (two eqv.)	1 : 2
7. Substrate to catalyst ratio	1 : 1
8. pH	9