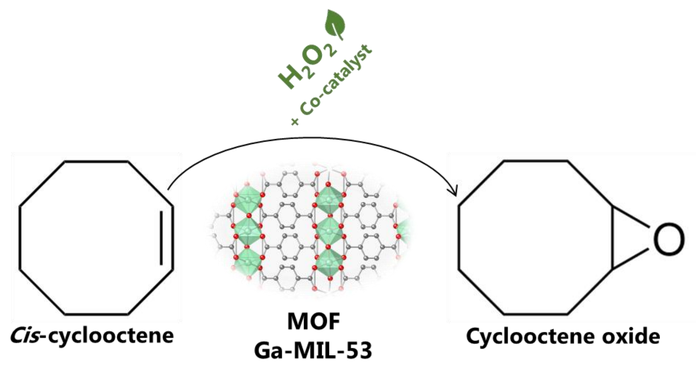
SYNTHESIS AND CHARACTERIZATION OF A ROBUST **GA-MOF CATALYST** FOR THE EPOXIDATION OF *CIS*-CYCLOOCTENE USING **H_2O_2 AS A GREEN OXIDANT**



Gabriela Tuono Martins XAVIER[1]*, Gustavo Felix BITENCOURT[1], Wagner Alves CARVALHO[1], Dalmo MANDELLI[1]

[1] Centro de Ciências Naturais e Humanas, Universidade Federal do ABC - UFABC, Av. dos Estados, 5001, Santo André – SP, 09210-580, Brazil.

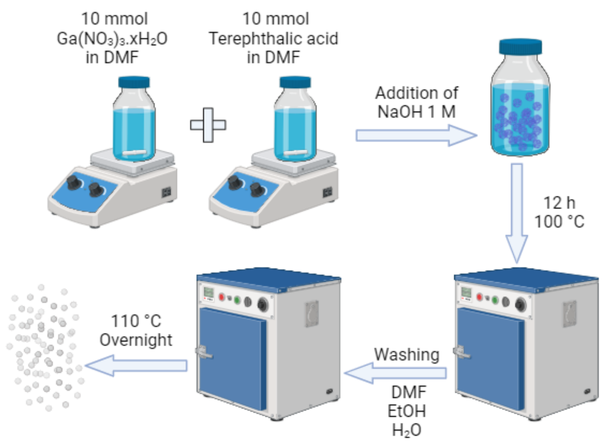
**Corresponding author: gabriela.xavier@ufabc.edu.br*

INTRODUCTION

An important route for producing epoxides, which are essential building blocks used in various industrial processes, is the catalytic oxidation of olefins [1]. Creating more sustainable and effective chemical procedures for these reactions is still a problem in modern chemistry. Because of their unique properties, using metal-organic frameworks (MOFs) as catalysts may present a viable alternative [2].

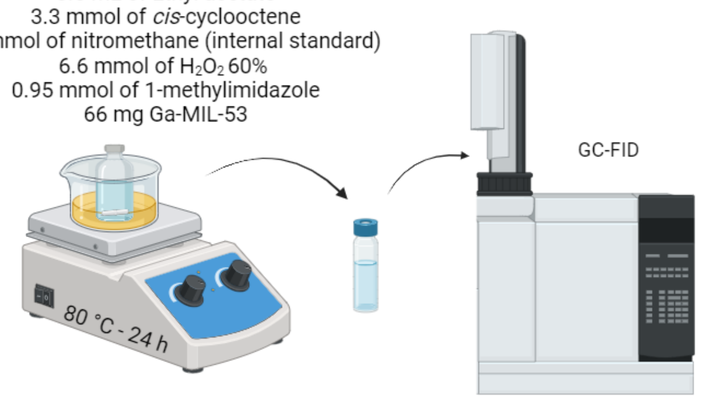
METHODS

Synthesis of Ga-MIL-53



Epoxidation of *cis*-cyclooctene

3.5 mL of Ethyl acetate
3.3 mmol of *cis*-cyclooctene
6.6 mmol of nitromethane (internal standard)
6.6 mmol of H_2O_2 60%
0.95 mmol of 1-methylimidazole
66 mg Ga-MIL-53



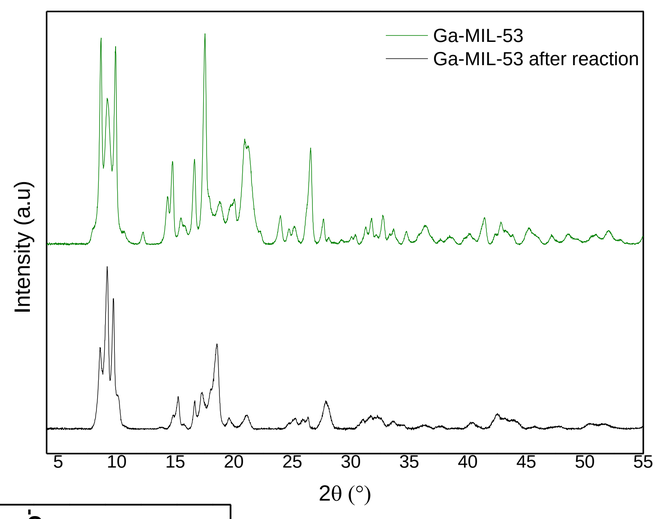
RESULTS

	C (%)	H (%)	N (%)	O (%)	Ga(%)
Chemical composition	38.6	2.4	-	33.9	25.1

Characterization of Ga-MOF

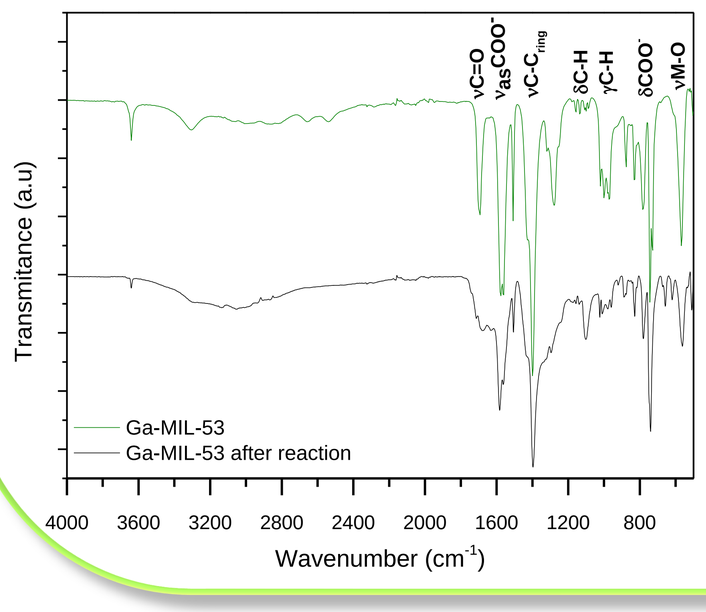
- XRD

Figure 1 - XRD pattern for Ga-MOF before (red) and after reaction (blue).



- FTIR

Figure 2 - FTIR spectra for Ga-MOF before (red) and after reaction (blue).



Catalytic performance – Epoxidation of *cis*-cyclooctene

Figure 3 – Kinetic profile of *cis*-cyclooctene epoxidation in 24 h of reaction. Reaction conditions: 66.6 mg of Ga-MIL-53, 0.95 mmol 1- methylimidazole, 3.5 mL of EtOAc, 3.3 mmol of *cis*-cyclooctene, 6.66 mmol of nitromethane, 6.66 mmol H_2O_2 60%. 80 °C

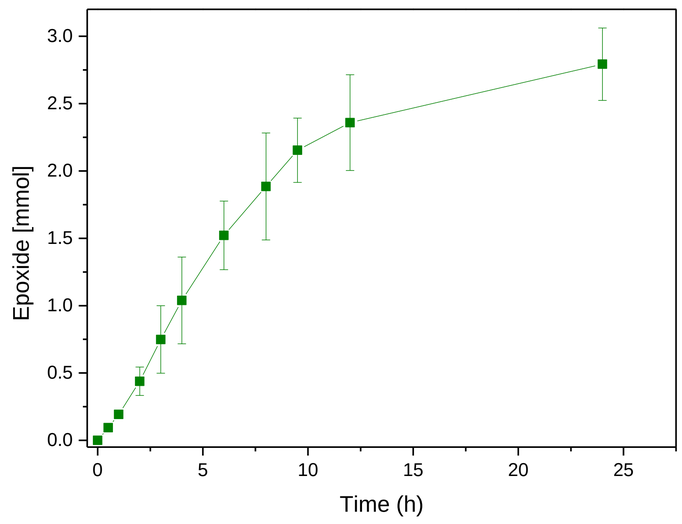


Table 1 – Conversion (%) and selectivity (%) of different cis-cyclooctene epoxidation reactions.

	Conversion (%)	Selectivity (%)
Blank	1.5	5.9
Ga-MIL-53	7.0	72.7
1-methylimidazole	16.9	52.3
Ga-MIL-53 + 1-methylimidazole	93.0	71.1
1° Cycle of reuse	81.6	93.0

- Heterogenous nature confirmed by Sheldon's test [4] after 2 h of reaction.

CONCLUSION

The Ga-MIL-53 was successfully synthesized and evaluated for its catalytic performance in olefin epoxidation. The obtained material demonstrated significant efficiency in olefin epoxidation, which increased with a cooperative metal-ligand approach in the presence of 1-methylimidazole. Ga-MIL-53 produced 2.4 mmol of the corresponding epoxide, with a conversion rate of 93%, and epoxide selectivity of 71%, using H_2O_2 as the oxidant.

REFERENCES

[1] Tombesi, A.; Pettinari, C.; *Inorganics* **2021**, 9.

[2] Aguirre-Díaz, L. M.; Reinares-Fisac, D.; Iglesias, M.; Gutiérrez-Puebla, E.; Gándara, F.; Snejko, N.; Monge, M. Á.; *Coord. Chem. Rev*. **2017**, 335, 1.

[3] Correia, G. A.; de Araújo, M. L.; Carvalho, W. A.; Sairre, M.; Cerchiaro, G.; Shul'pina, L. S.; Kozlov, Y. N.; Shul´pin, G. B.; Kirillov, A. M.; Mandelli, D.*; Mol. Catal*. **2022**, 528, 112457.

[4] Lempers, H. E. B.; Sheldon, R. A.; *J. Catal.* **1998**, 175, 62.