Reaction Mechanism of the Isomerization of Monoterpene Epoxides with Fe^{3+}: A Computational Approach

SUPPLEMENTARY INFORMATION

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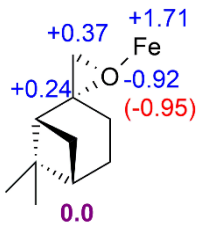
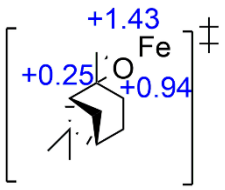
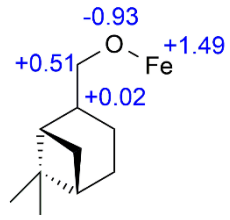
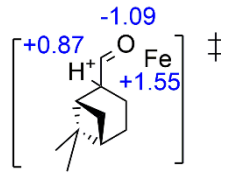
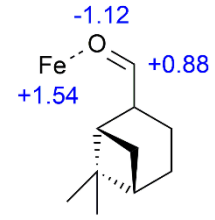
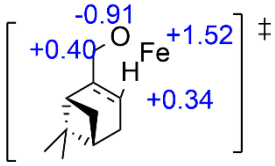
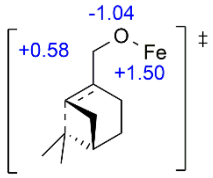
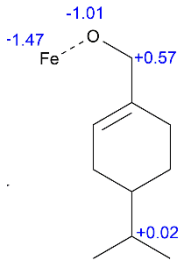
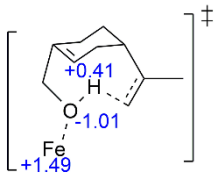
General description: Herein, we present the values of the Laplacian of the electronic density ($\nabla^2\rho(r_b)$) and the $|V(r_b)|/G(r_b)$ ratio at the bond critical point of the Fe-O bond for all structures generated towards the determination of the reaction mechanism of both epoxides. It is important taking into account that in the case of β-pinene epoxide, all intermediate and transition states were elucidated while in the case of α-pinene epoxide only intermediates were determined without finding the transition states that connect those structures.

Table S1. Topological properties of the Fe-O interaction of all structures involved during the proposed rearrangement of β-pinene epoxide.

Structure	$\nabla^2\rho(r_b)$ (a.u)	$\|V(r_b)\|/G(r_b)$ (a.u)
	4.62E-14	1.03
	-0.17	1.042

	1.55E-15	1.15
	4.09E-16	1.048
	6.46E-16	-1.046
	8.84E-15	1.11
	5.03E-17	1.12
	5.10E-15	1.13
	2.48E-13	1.12

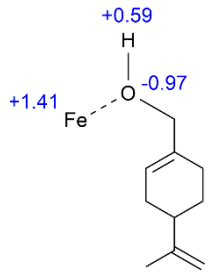
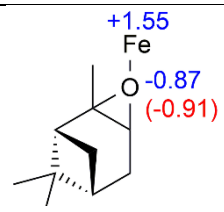
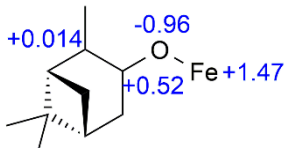
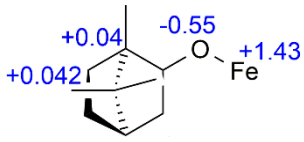
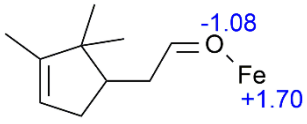
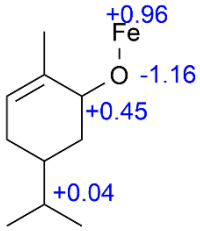
	2.78E-16	1.02

Table S2. Topological properties of the Fe-O interaction of all structures involved during the proposed rearrangement of **α**-pinene epoxide.

Structure	$\nabla^2\rho(r_b)$ (a.u)	$\lvert V(r_b)\rvert/G(r_b)$ (a.u)
	3.23E-16	1.04
	1.29E-14	1.12
	7.72E-17	1.07
	1.74E-16	1.06
	4.79E-15	1.08

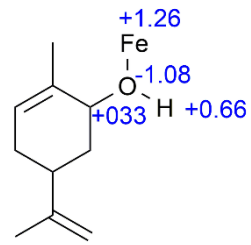
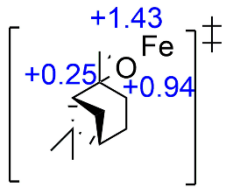
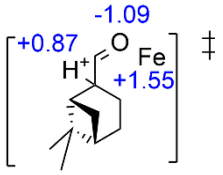
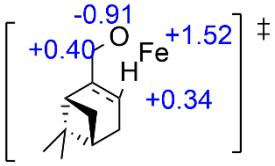
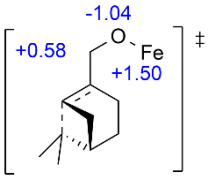
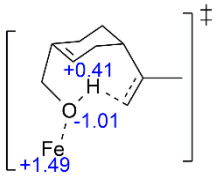
	1.84E-15	1.04

Table S3. Imaginary frequencies of the different transition states

Structure	$\boldsymbol{Frequence}$ $(\boldsymbol{cm^{-1}})$
	-162.48
	-183.05
	-1584.11
	-157.52
	-1368.08