

# Supplementary Information

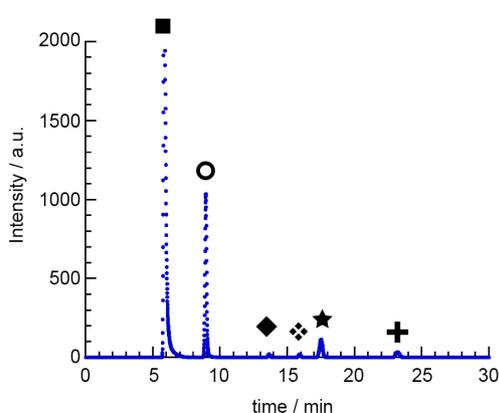
## AuNP@TiO<sub>2</sub> Catalyzed Peroxidation of Ethyl- and *n*-Propylbenzene: Exploring the Interaction Between Radical Species and the Nanoparticle Surface

Charles-Oneil L. Crites,<sup>a</sup> José Carlos Netto-Ferreira,<sup>\*,a,b</sup> Geniece L. Hallett-Tapley<sup>c</sup> and Juan Cesar Scaiano<sup>\*,a</sup>

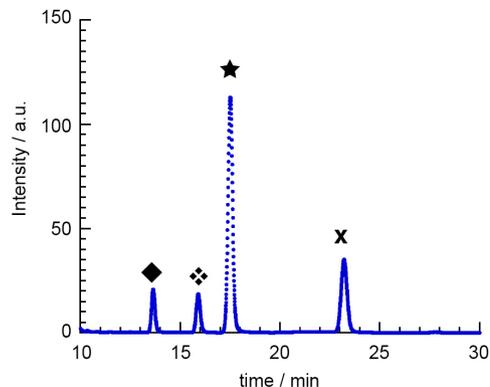
<sup>a</sup>Centre for Catalysis Research and Innovation, Department of Chemistry and Biomolecular Sciences, University of Ottawa, 10 Marie Curie, K1N 6N5 Ottawa, Canada

<sup>b</sup>Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), Av. Nossa Senhora das Graças 50, 25520-020 Rio de Janeiro-RJ, Brazil

<sup>c</sup>Department of Chemistry, St. Francis Xavier University, P.O. Box 5000, B2G 2W5 Antigonish, Canada



**Figure S1.** Representative HPLC trace for the peroxidation of ethylbenzene in the presence of CHP initiator. Peak identification: ethylbenzene and cumene (■); acetophenone (○); CHP (◆); ethylbenzene hydroperoxide (⋄); cumyl alcohol (★) and *sec*-phenethyl alcohol (⊕).

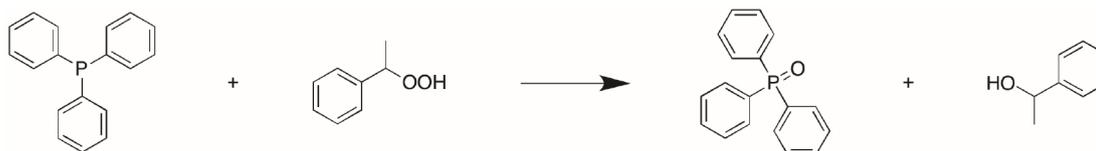


**Figure S2.** Expanded view of the representative HPLC trace of the peroxidation of ethylbenzene in the presence of initiator (CHP). Peak identification: CHP (◆); ethylbenzene hydroperoxide (⋄); cumyl alcohol (★) and *sec*-phenethyl alcohol (⊕).

Determination of the calibration factor of ethylbenzene hydroperoxide and propylbenzene hydroperoxide

Calibration curves were used to determine the concentration of all compounds (cumyl alcohol, acetophenone, 1-phenethyl alcohol and cumene hydroperoxide). However, due to the unstable nature of the ethylbenzene hydroperoxide, isolation was not possible.

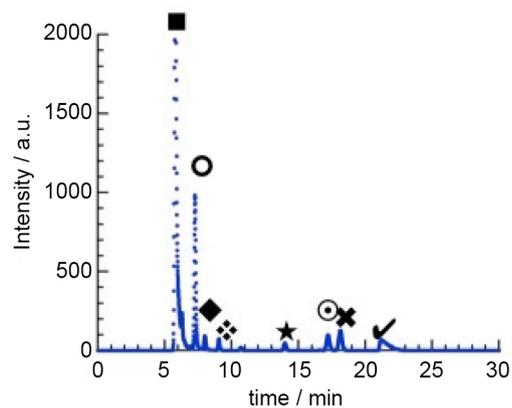
The calibration factor of ethylbenzene hydroperoxide was determined by quenching the hydroperoxide using triphenylphosphine to observe the formation of *sec*-phenethyl alcohol as the quenching product. Knowing the concentration of *sec*-phenethyl alcohol before and after quenching allows for a calculation of the calibration factor of the ethylbenzene hydroperoxide compared to the calibration factor of the *sec*-phenethyl alcohol.



**Scheme S1.** Quenching of ethylbenzene hydroperoxide by triphenylphosphine producing the corresponding alcohol (*sec*-phenethyl alcohol) and triphenylphosphine oxide.

\*e-mail: josecarlos@photo.chem.uottawa.ca,  
scaiano@photo.chem.uottawa.ca

This manuscript is dedicated to Frank Herbert Quina.

Peroxidation of *n*-propylbenzene

**Figure S3.** Representative HPLC trace of the peroxidation of *n*-propylbenzene. Peak identification: propylbenzene and cumene (■); propiophenone (○); benzaldehyde (◆); acetophenone (◆); cumene hydroperoxide (★); 1-phenyl-1-propanol (⊙); cumyl alcohol (x) and unknown product (✓).