

[Home](#)[Online Library ACP](#)

- Recent Final Revised Papers
- [Volumes and Issues](#)
- Special Issues
- Library Search
- Title and Author Search

[Online Library ACPD](#)[Alerts & RSS Feeds](#)[General Information](#)[Submission](#)[Review](#)[Production](#)[Subscription](#)[Comment on a Paper](#)

Impact  
Factor  
4.865

ISI  
indexed

[Volumes and Issues](#) [Contents of Issue 6](#)

Atmos. Chem. Phys., 3, 1999-2014, 2003

[www.atmos-chem-phys.net/3/1999/2003/](http://www.atmos-chem-phys.net/3/1999/2003/)

© Author(s) 2003. This work is licensed under a Creative Commons License.

## Measurements of photo-oxidation products from the reaction of a series of alkyl-benzenes with hydroxyl radicals during EXACT using comprehensive gas chromatography

J. F. Hamilton<sup>1</sup>, A. C. Lewis<sup>2</sup>, C. Bloss<sup>1</sup>, V. Wagner<sup>1</sup>, A. P. Henderson<sup>3</sup>, B. T. Golding<sup>3</sup>, K. Wirtz<sup>4</sup>, M. Martin-Reviejo<sup>4</sup>, and M. J. Pilling<sup>1</sup>

<sup>1</sup>University of Leeds, Department of Chemistry, Woodhouse Lane, Leeds, LS2 9JT, UK

<sup>2</sup>University of York, Department of Chemistry, Heslington, York, YO10 5DD, UK

<sup>3</sup>School of Natural Sciences – Chemistry, Bedson Building, University of Newcastle upon Tyne, Newcastle upon Tyne NE1 7RU, UK

<sup>4</sup>Fundación Centro de Estudios Ambientales del Mediterráneo (CEAM), EUPHORE laboratories, C/Charles Darwin, 14-Parc Tecnológico, Paterna, Valencia, Spain

**Abstract.** Photo-oxidation products from the reaction of a series of alkyl-benzenes, (benzene, toluene, *p*-xylene and 1,3,5-trimethyl-benzene) with hydroxyl radicals in the presence of NO<sub>x</sub> have been investigated using comprehensive gas chromatography (GCxGC). A GCxGC system has been developed which utilises valve modulation and independent separations as a function of both volatility and polarity. A number of carbonyl-type compounds were identified during a series of reactions carried out at the European Photoreactor (EUPHORE), a large volume outdoor reaction chamber in Valencia, Spain. Experiments were carried as part of the EXACT project (Effects of the oXidation of Aromatic Compounds in the Troposphere). Two litre chamber air samples were cryo-focused, with a sampling frequency of 30 minutes, allowing the evolution of species to be followed over oxidation periods of 3-6 hours. To facilitate product identification, several carbonyl compounds, which were possible products of the photo-oxidation, were synthesised and used as reference standards.

For toluene reactions, observed oxygenated intermediates found included the co-eluting pair  $\alpha$ -angelicalactone/4-oxo-2-pentenal, maleic anhydride, citraconic anhydride, benzaldehyde and *p*-methyl benzoquinone. In the *p*-xylene experiment, the products identified were E/Z-hex-3-en-2,5-dione and citraconic anhydride. For 1,3,5-TMB reactions, the products identified were 3,5-dimethylbenzaldehyde, 3,5-dimethyl-3H-furan-2-one and 3-methyl-5-methylene-5H-furan-2-one. Preliminary quantification was carried out on identified compounds using liquid standards. Comparison of FTIR and GCxGC for the measurement of the parent aromatics generally showed good agreement. Comparison of the concentrations observed by GCxGC to concentration-time profiles simulated using the Master Chemical Mechanism, MCMv3, demonstrates that this mechanism significantly over-predicts the concentrations of many product compounds and highlights the uncertainties which exist in our understanding of the atmospheric oxidation of aromatics.

[Search ACP](#)

Library Search

Author Search

[News](#)

- Sister Journals AMT & GMD
- Financial Support for Authors
- Journal Impact Factor
- Public Relations & Background Information

[Recent Papers](#)

01 | ACP, 11 Mar 2009:  
Measurements of Pollution In  
The Troposphere (MOPITT)  
validation through 2006

02 | ACP, 11 Mar 2009:  
Air-sea fluxes of biogenic  
bromine from the tropical  
and North Atlantic Ocean

03 | ACPD, 10 Mar 2009:  
Characterization of organic  
ambient aerosol during  
MIRAGE 2006 on three  
platforms

04 | ACPD, 10 Mar 2009:  
Regional differences in

■ [Final Revised Paper \(PDF, 360 KB\)](#) ■ [Discussion Paper \(ACPD\)](#)

Citation: Hamilton, J. F., Lewis, A. C., Bloss, C., Wagner, V., Henderson, A. P., Golding, B. T., Wirtz, K., Martin-Reviejo, M., and Pilling, M. J.: Measurements of photo-oxidation products from the reaction of a series of alkyl-benzenes with hydroxyl radicals during EXACT using comprehensive gas chromatography, *Atmos. Chem. Phys.*, 3, 1999-2014, 2003. ■ [Bibtex](#) ■ [EndNote](#) ■ [Reference Manager](#)