

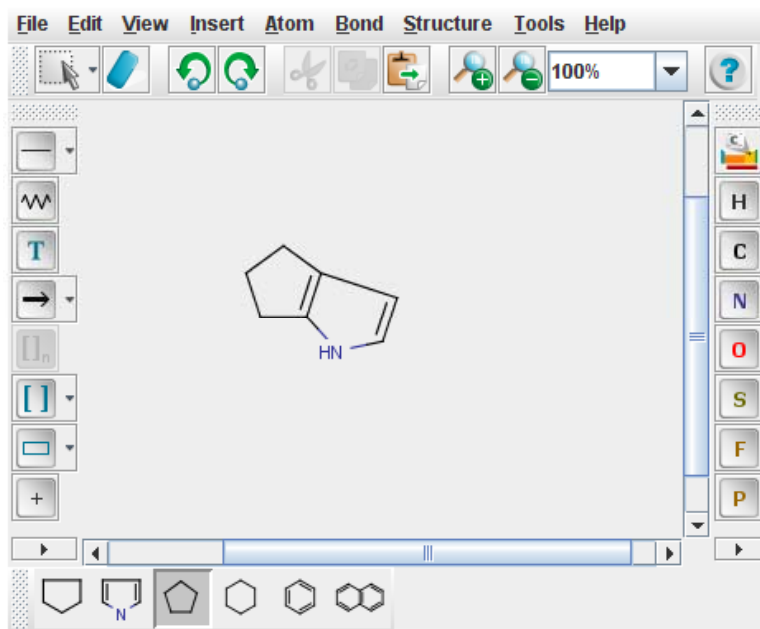
# Computer Modeling

## New & Improved ClogP calculator

This calculator correctly adjusts for charged parts of molecules.

How to use it:

1. Build a structure using the bond and ring buttons as usual.
  - To change an atom from carbon to another atom, click on the appropriate letter in the upper left of the panel. Then click on the atom you want to change.
  - To change the charge of an atom, click on the + or - buttons.
2. Choose "logP" from the "Tools" menu.
  - A window will appear with the logP value.
  - NOTE:The first time you calculate logP, it will take a little while to load the plug-in; please be patient.



Early example Clog P  
Calculated logarithm of the  
water/octanol partition coefficient

<http://intro.bio.umb.edu/111-112/OLLM/111F98/newclogp.html>

# Smiles

## SIMPLIFIED MOLECULAR INPUT LINE ENTRY SYSTEM

Allows entry of chemical structures into  
computer programs to predict  
properties

# Example

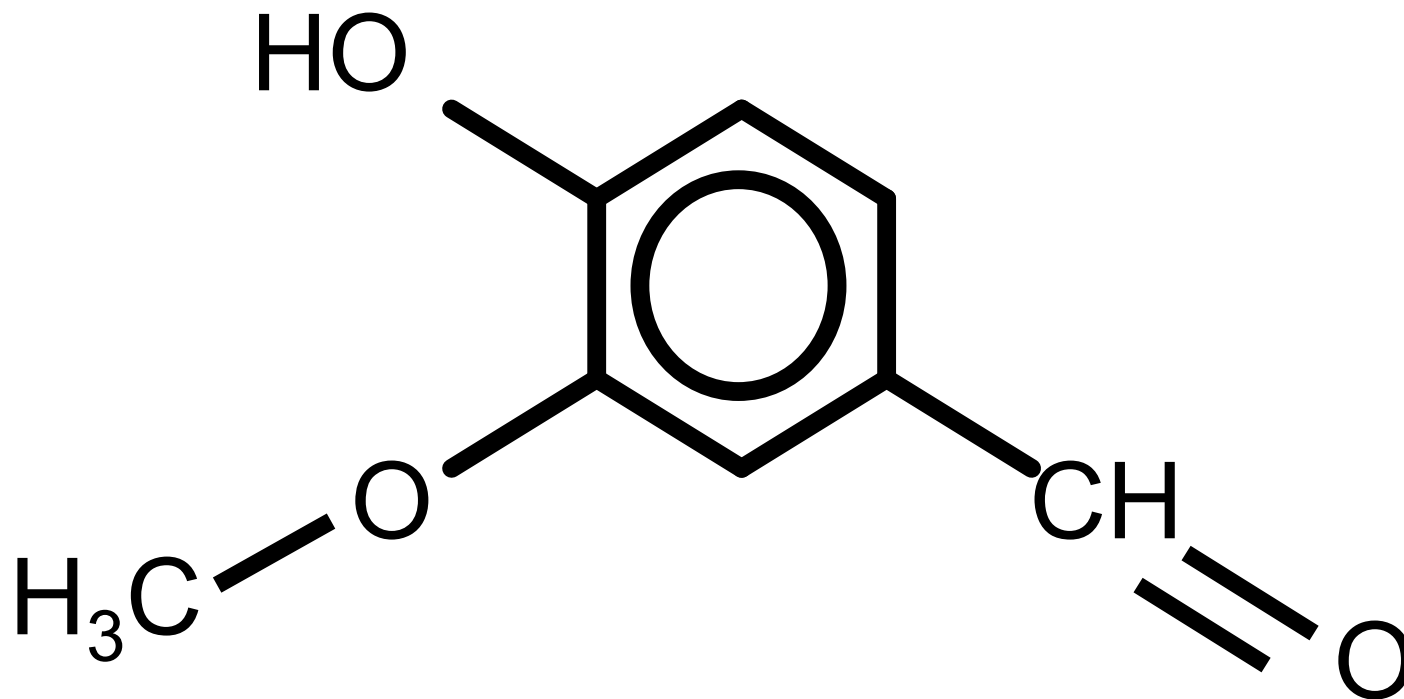
Case Important-  
Aliphatic Upper Case  
Aromatic Lower Case  
Hydrogen Not Included

SINGLE BOND C-C  
DOUBLE BOND C=C  
TRIPLE BOND C#C

Rings- # at start and end  
e.g. c1ccccc1Br is Bromobenzene

# Smiles Vanilin

COc1cc(C=O)ccc1O



## Using the PBT Profiler

[Information needed](#)  
[Examples](#)  
[Interpreting Results](#)  
[What's new?](#)

## Related Links

[About PBTs](#)  
[PBT Strategy](#)  
[TRI PBT Project](#)  
[P2 Framework](#)  
[Links & Contacts](#)



Comments

Persistent, Bioaccumulative, and Toxic Profiles Estimated for Organic Chemicals On-Line

# PBT Profiler

A Component of OPPT's  
P2 Framework

*Assessing Chemicals in  
the Absence of Data*

[About](#)  
[Methodology](#)  
[Criteria](#)  
[Anonymity & Security](#)  
[Definitions](#)  
[Terms of Use](#)  
[Chemicals That  
Can't be Profiled](#)

The PBT Profiler was developed as a voluntary screening tool to identify Pollution Prevention opportunities for chemicals without experimental data.

Users of the PBT Profiler acknowledge that they have read and accept the [Terms of Use](#)

[Start the PBT Profiler](#)

*Developed by the [Environmental Science Center](#) under contract to the [Office of Pollution Prevention and Toxics](#), U.S. [Environmental Protection Agency](#)*

*Computer Resources Donated by [Syracuse Research Corporation](#)*

*Ver 1.203*

*Last Updated September 21, 2006*

[www.pbtprofiler.net](http://www.pbtprofiler.net)

# Vanillin

## Results

Orange or red highlights indicate that the EPA [criteria](#) have been exceeded.

[Black-and-white version](#)

Persistence

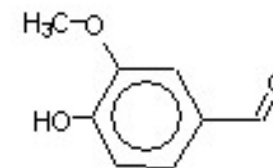
Bioaccumulation

Toxicity

121-33-5 Benzaldehyde, 4-hydroxy-3-methoxy-

PBT Profiler Estimate = **PBT**

<u>Media</u>	<u>Half-Life</u> (days)	<u>Percent in</u> <u>Each Medium</u>	<u>BCF</u>	<u>Fish ChV</u> (mg/l)
Water	15	33%	1.7	0.48
Soil	30	67%		
Sediment	140	0%		
Air	0.58	0%		



[P2 Considerations and more information](#)

EPI v3.20

File Edit Functions BatchMode ShowStructure Output Fugacity STP Other Help

PhysProp Previous Get User Save User CAS Input **CALCULATE** ClearInputField What's New

Enter SMILES:

Chem NAME:

NameLookup

Henry LC (atm-m<sup>3</sup>/mole):  Wat Sol (mg/L):  MP:

Vap Pr (mm Hg):  BP:

River:  Lake:  Log Kow :

Water Depth (meters):  1


Wind Velocity (m/sec):  5

Current Velocity(m/sec):  1

Output

Summary

Full



The Estimation Programs Interface (EPI) Suite™ was developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). It is a screening-level tool and cannot be used for all chemical substances. Like other such tools, it is intended for use in screening level applications such as to quickly screen chemicals for release potential, and "bin" chemicals by priority for future work. Estimated values should not be used when experimental (measured) values are available.

Important information on the performance, development and application of the individual estimation programs within EPI Suite™ is included in the User's Guide.

© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.

# EPI Suite

start Steve Herman - Inbo... EPI v3.20 11:48 AM

# Fugacity Level III

## Level III Results

Vanillin

Chemical Type 1

Mass Balance

Fugacity

Phase Properties

Advection

Reaction

Intermedia Transport

Individual Process D Values

Bulk Compartment

Fugacity

VZ

Pa

mol/Pa

Air

4.76E-09

1.40E+12

Water

1.70E-07

1.16E+13

Soil

1.67E-08

6.62E+15

Sediment

1.59E-06

2.36E+13

# Environmental Profile

## Biodegradation

EPA models predict that most major components will biodegrade in weeks.

## Atmospheric Oxidation

Model predict that this will be rapid, with  $\frac{1}{2}$  lives ranging from less than 1 to 7 hours for major components.



Analysis based on models and informed assumptions.

# Environmental Profile

## **Fugacity**

The EPA's Level 3 fugacity model predicts ~90% of the formulation will partition to sediment where Biodegradation will take place over several weeks.

## **Acute and Chronic Aquatic Toxicity**

Expected to be low, given the low water solubility of most components.

## Designing Small Molecules for Biodegradability

R. S. Boethling,<sup>\*,†</sup> Elizabeth Sommer,<sup>‡</sup> and David DiFiore<sup>‡</sup>

U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics 7406M, 1200 Pennsylvania Avenue, NW, Washington, DC 20460

Received September 14, 2006

### Contents

1. Introduction	2207
2. Scope of this Work	2208
3. Environment, Structure, and Biodegradability	2208
4. Rules of Thumb	2209
5. Designing Biodegradable Chemicals: Ten Examples	2210
5.1. Alkylbenzene Sulfonates	2210
5.2. Dialkyl Quaternaries	2211
5.3. Chelants/Sequestrants	2212
5.4. Drilling Base Fluids	2212

options. The PPA established a national policy that pollution should be prevented or reduced at the source whenever feasible, pollution that cannot be prevented should be recycled in an environmentally safe manner whenever feasible, pollution that cannot be prevented or recycled should be treated in an environmentally safe manner whenever feasible, and disposal or other release into the environment should be employed only as a last resort and should be conducted in an environmentally safe manner.

The Act defines source reduction as any practice that "(i) reduces the amount of any hazardous substance...prior to recycling, treatment or disposal; and (ii) reduces the hazards

Musks- ester linkages good, also ketone and oxygen (but not aliphatic ether), hydrocarbons bad

Boethling et al

# NIOSH Studies

## Chemistry of Indoor Environments

Ray Wells

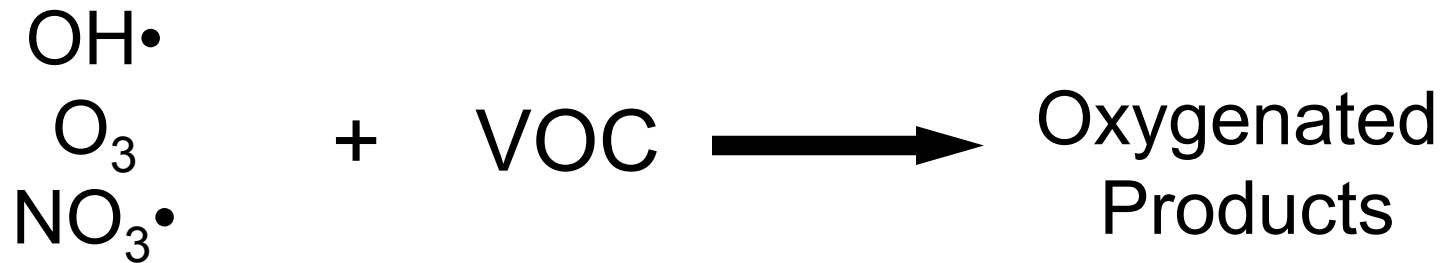
Exposure Assessment Branch  
NIOSH  
Morgantown, WV

# Indoor Reactants

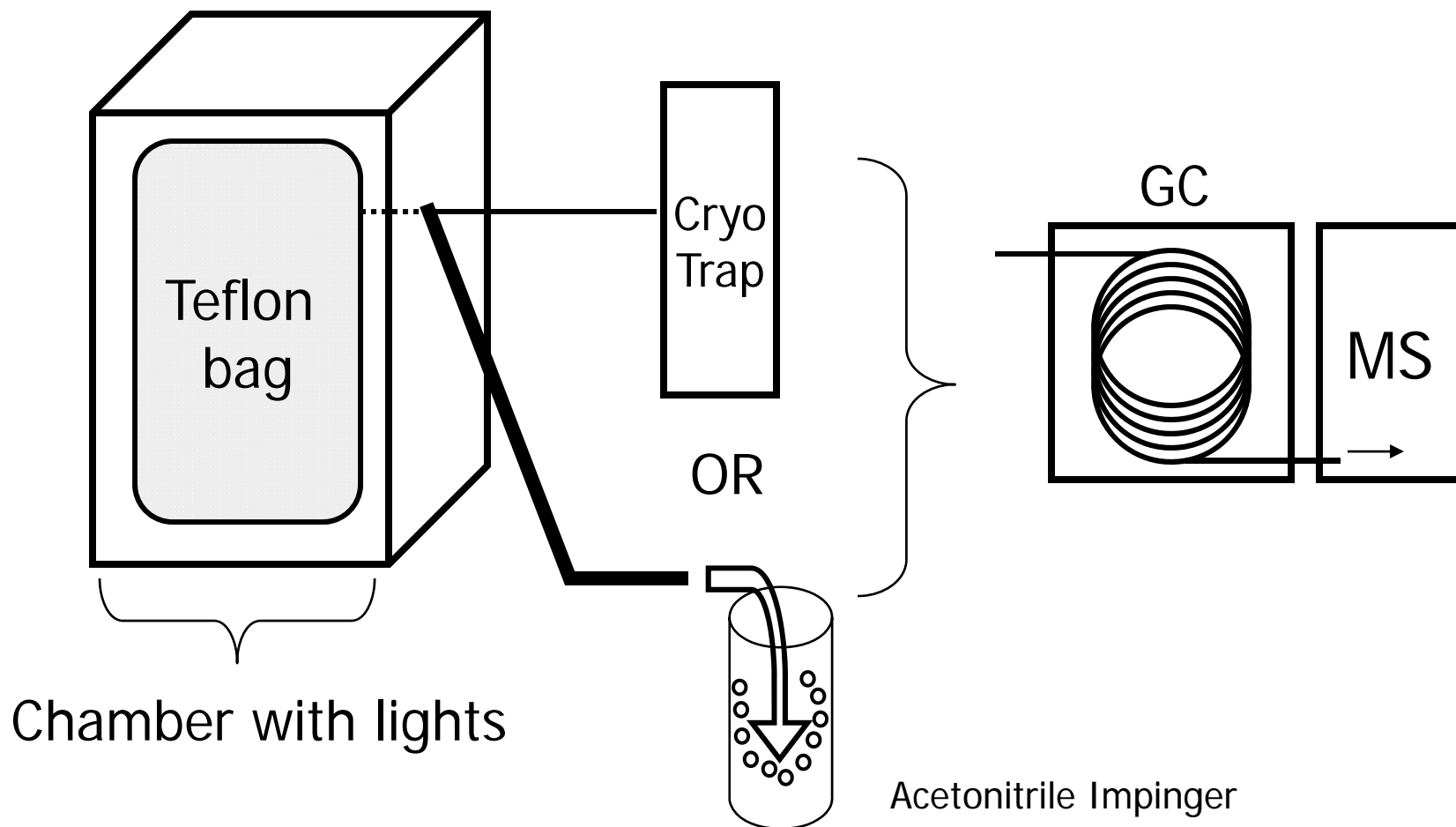
Hydroxyl Radical (OH•)

Ozone (O<sub>3</sub>)

Nitrate Radical (NO<sub>3</sub>•)

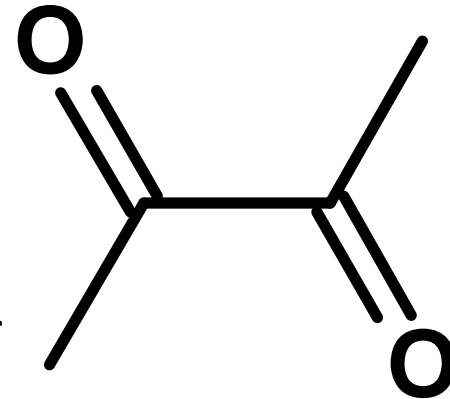


# Experimental

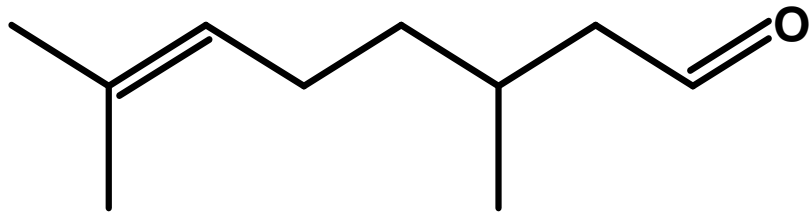


# Diacetyl

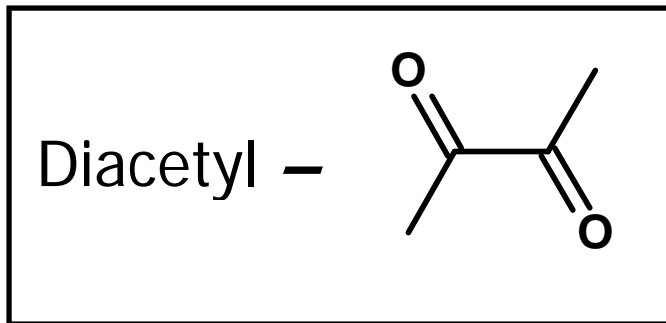
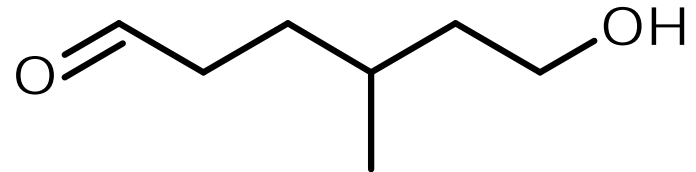
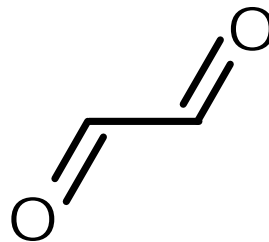
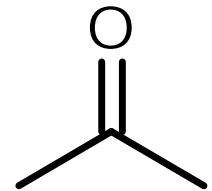
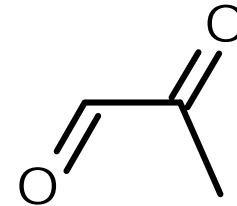
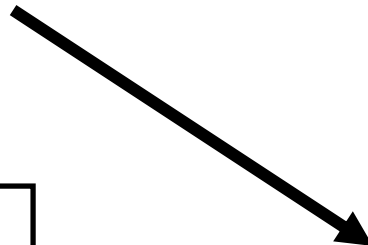
- Small oxygenated organic
- Microwave popcorn workers  
Kanwal, et al. (2006) J of Occup Env Med 48 149-157.
- Rat exposures – airway damage  
Hubbs, et al. (2002) Tox Appl Pharma 185 128-135.



# Citronellal and O<sub>3</sub>

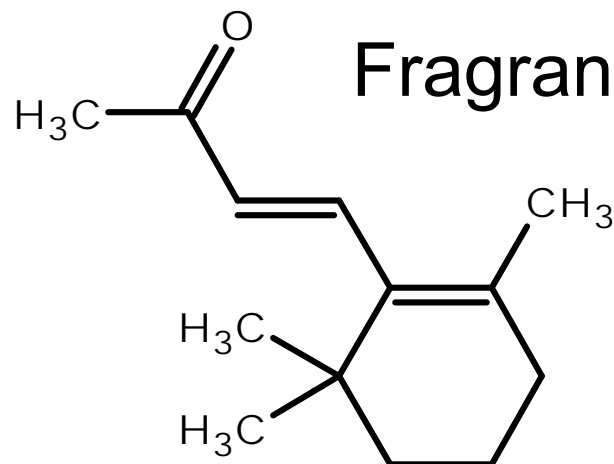


+ Reactant

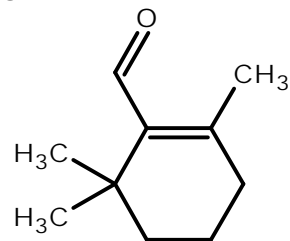
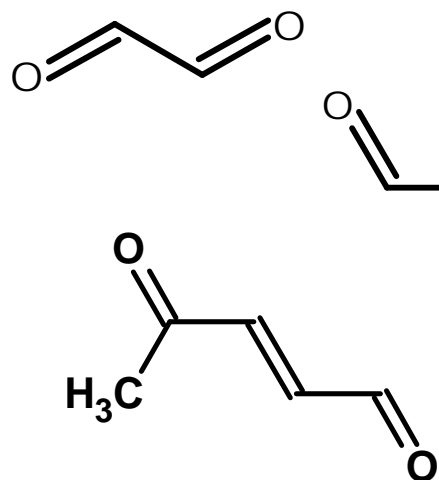
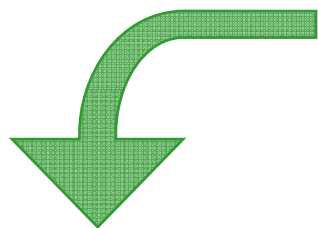


# $\beta$ -IONONE + OH/O<sub>3</sub>

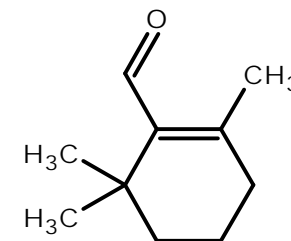
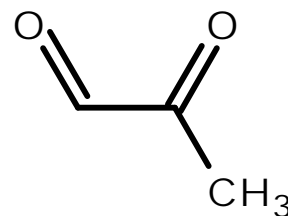
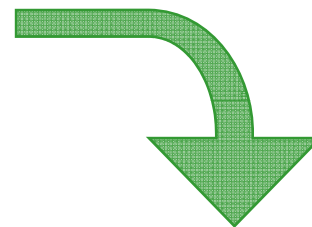
Fragrance additive (violets)



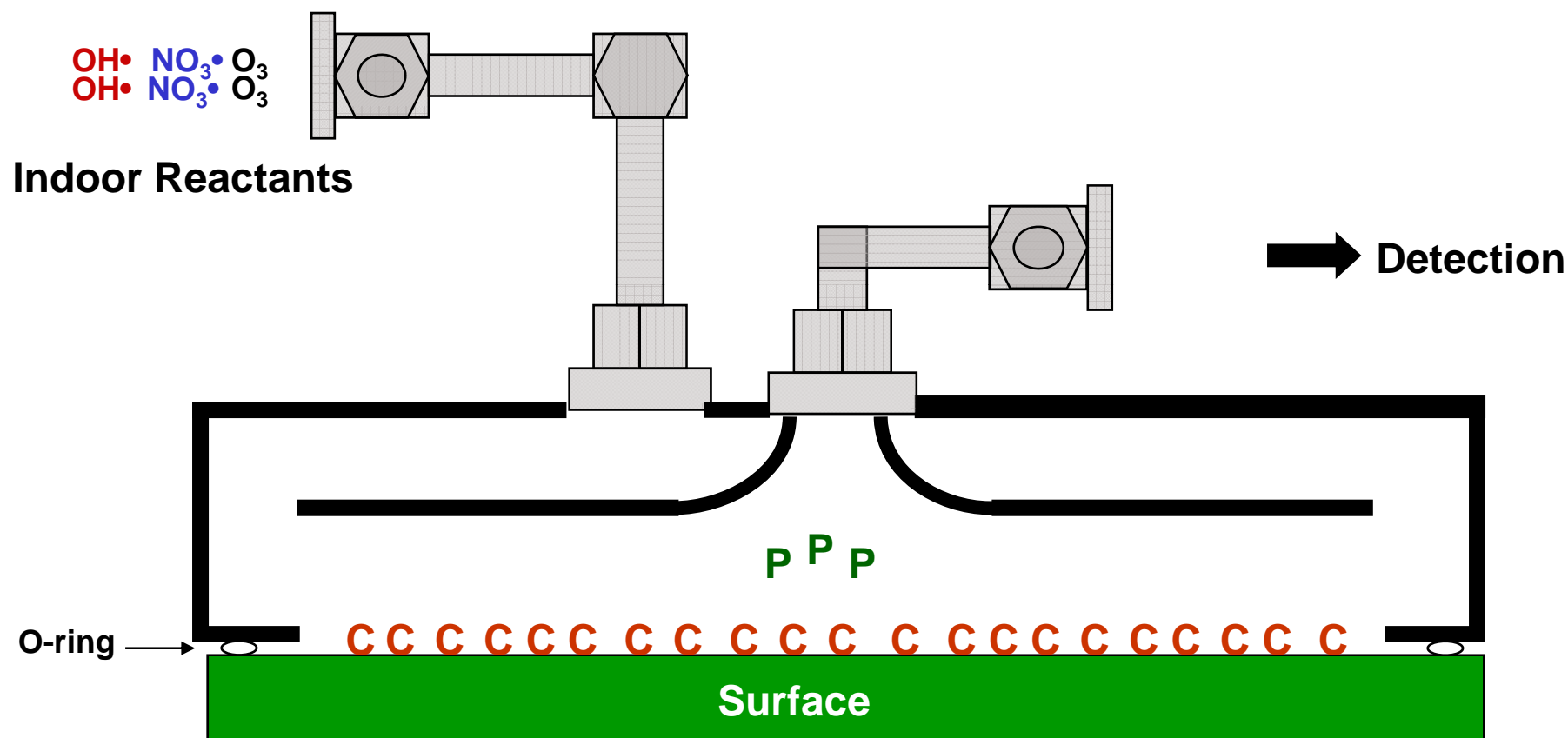
+ OH•



+ O<sub>3</sub>

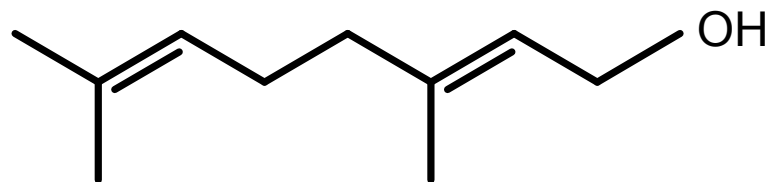


# Surface Chemistry



**C = chemical applied to surface**

**P = products formed after reaction with surface chemicals**



Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

SCIENCE @ DIRECT®

Atmospheric Environment 40 (2006) 726–735



ELSEVIER

ATMOSPHERIC  
ENVIRONMENT

[www.elsevier.com/locate/atmosenv](http://www.elsevier.com/locate/atmosenv)

# Gas-phase chemistry of citronellol with ozone and OH radical: Rate constants and products

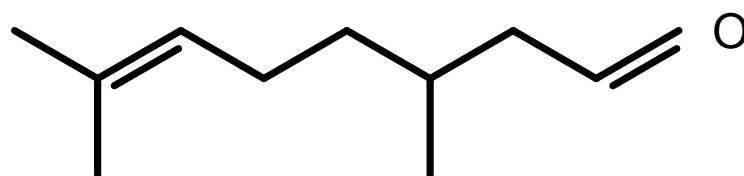
Jason E. Ham<sup>a</sup>, Steven P. Proper<sup>b</sup>, J.R. Wells<sup>a,\*</sup>

<sup>a</sup>*Exposure Assessment Branch, Health Effects Laboratory Division, National Institute for Occupational Safety and Health,  
1095 Willowdale Road, Morgantown, WV 26505, USA*

<sup>b</sup>*Department of Science and Mathematics, Environmental Chemistry, Kettering University, 1700 West Third Avenue, Flint, MI 48504, USA*

Received 4 August 2005; received in revised form 4 October 2005; accepted 4 October 2005

Products      acetone  
                  ethanedial  
                  2-oxopropanal



Available online at [www.sciencedirect.com](http://www.sciencedirect.com)



Atmospheric Environment 41 (2007) 4482–4491

---

---

**ATMOSPHERIC  
ENVIRONMENT**

---

---

[www.elsevier.com/locate/atmosenv](http://www.elsevier.com/locate/atmosenv)

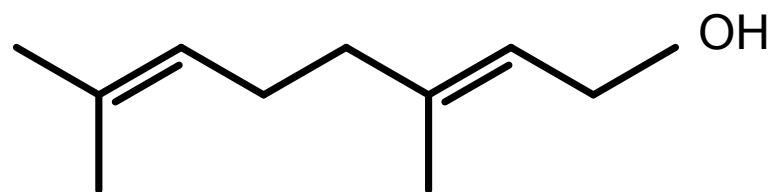
## Citronellal reactions with ozone and OH radical: Rate constants and gas-phase products detected using PFBHA derivatization

J.C. Harrison, J.E. Ham, J.R. Wells\*

*Exposure Assessment Branch, Health Effects Laboratory Division, National Institute for Occupational Safety and Health,  
1095 Willowdale Road Morgantown, WV 26505, USA*

Received 20 October 2006; received in revised form 21 December 2006; accepted 17 January 2007

**Products** 3-methylhexanediol  
2-oxopropanal



Available online at [www.sciencedirect.com](http://www.sciencedirect.com)



Atmospheric Environment 41 (2007) 1188–1199

---

---

**ATMOSPHERIC  
ENVIRONMENT**

---

---

[www.elsevier.com/locate/atmosenv](http://www.elsevier.com/locate/atmosenv)



**ELSEVIER**

# Geraniol (2,6-dimethyl-2,6-octadien-8-ol) reactions with ozone and OH radical: Rate constants and gas-phase products

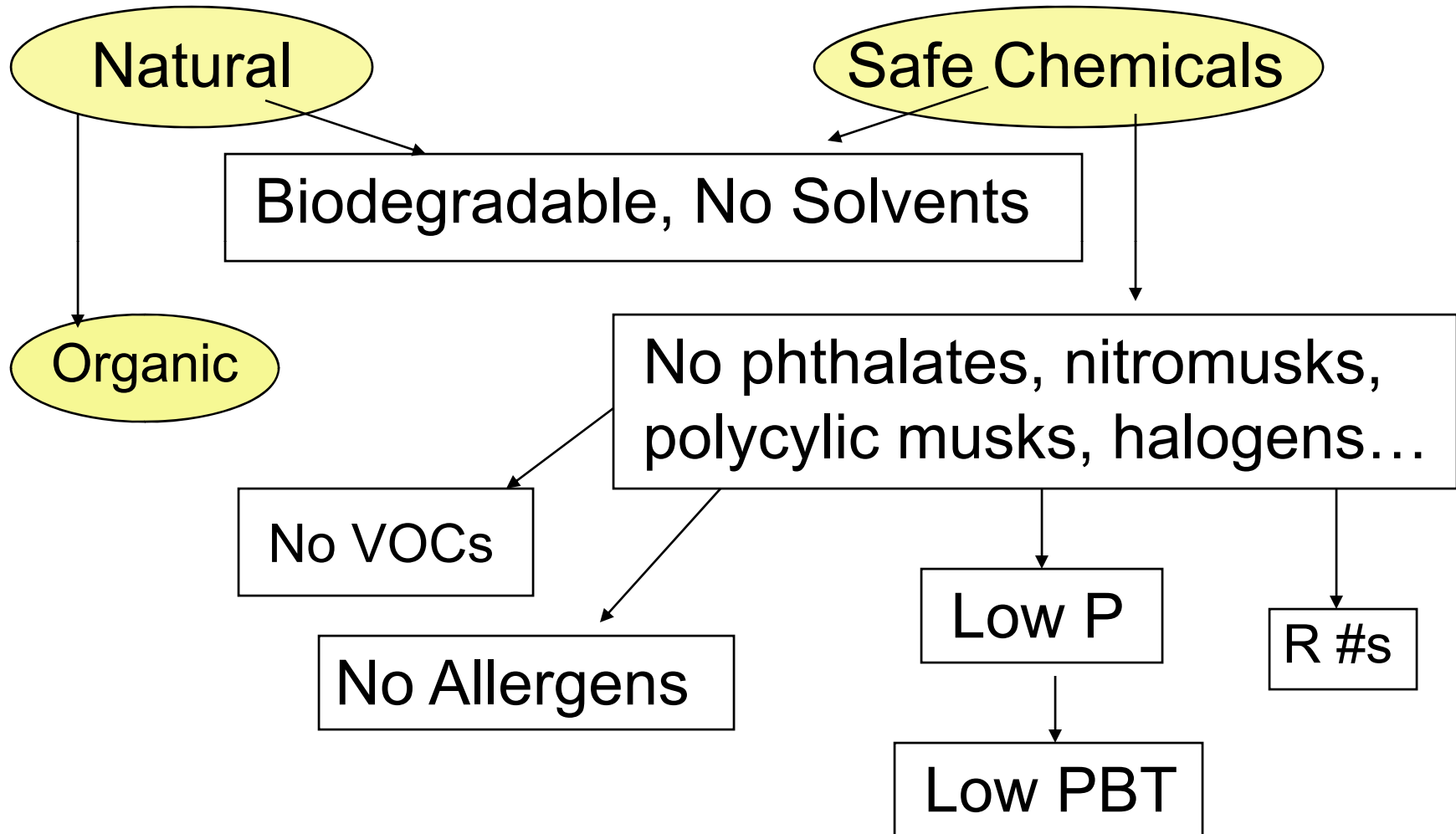
Crystal D. Forester, Jason E. Ham, J.R. Wells\*

*Exposure Assessment Branch, Health Effects Laboratory Division, National Institute for Occupational Safety and Health,  
1095 Willowdale Road, Morgantown, WV 26505, USA*

Received 29 August 2006; received in revised form 15 September 2006; accepted 22 September 2006

**Products**      acetone  
                         hydroxyacetaldehyde  
                         ethanedial  
                         2-oxopropanal

# Conceptual Green Algorithm



# H L Mencken



For every complex question  
there is a simple answer-  
and its wrong.

Thanks  
For  
Your  
Attention

