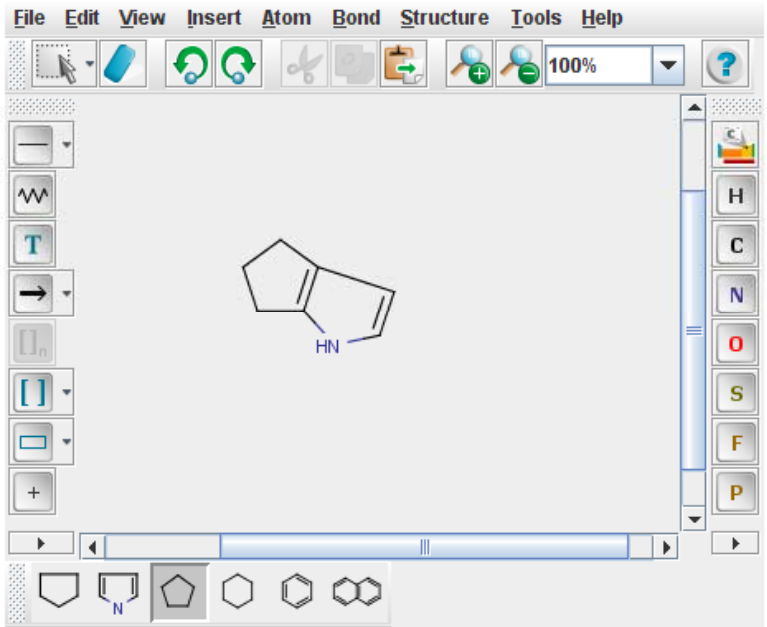
Computer Modeling

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

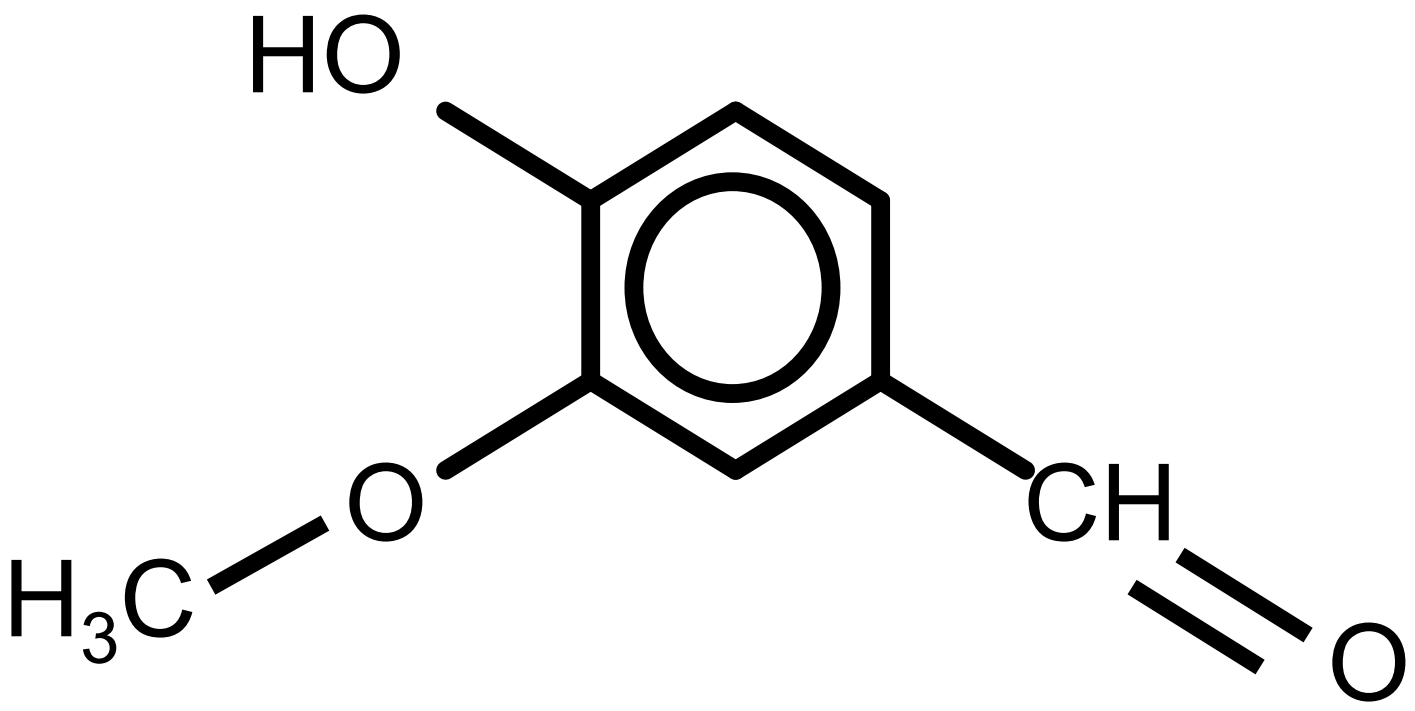
Case Important-
Aliphatic Upper Case
Aromatic Lower Case
Hydrogen Not Included

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

Vanillin

Results

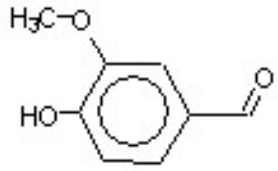
Orange or red highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

Persistence			Bioaccumulation	Toxicity

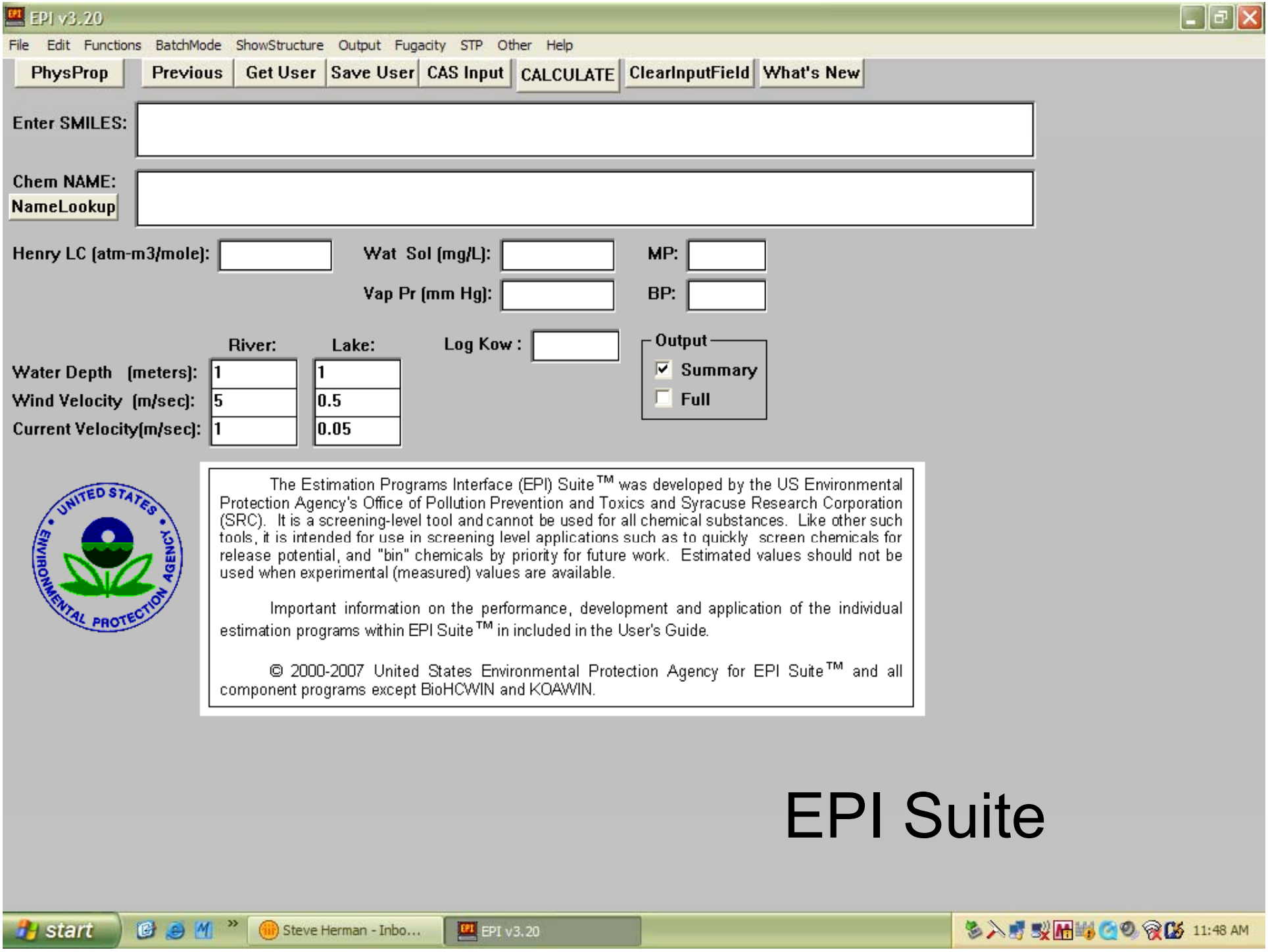
121-33-5 Benzaldehyde, 4-hydroxy-3-methoxy-

PBT Profiler Estimate = PBT

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

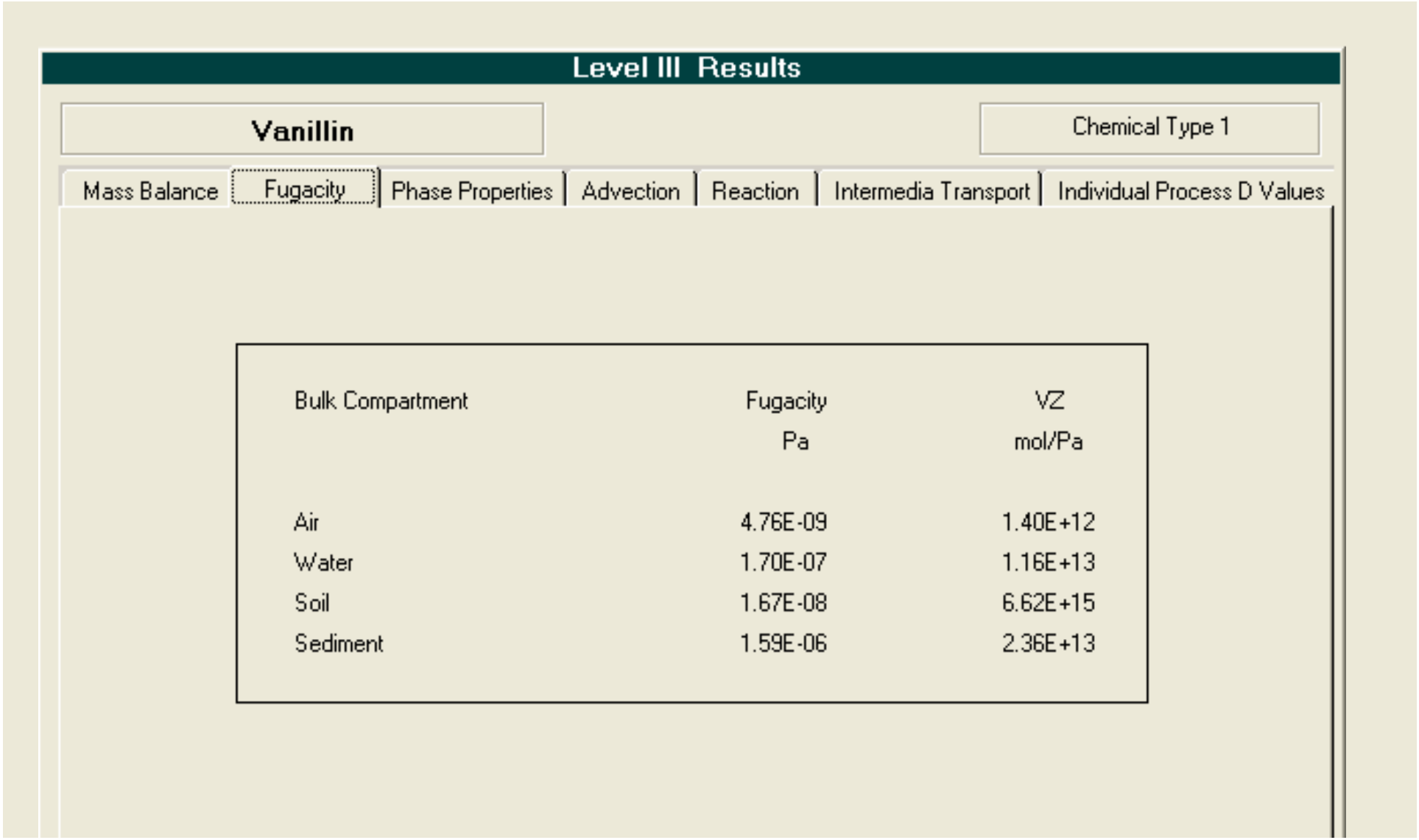


P2 Considerations and more information


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-m3/mole):
Wat Sol (mg/L):
MP:
Vap Pr (mm Hg):
BP:
River:
Lake:
Log Kow :
Output
Summary
Full
Water Depth (meters):
Wind Velocity (m/sec):
Current Velocity(m/sec):
1
5
1
1
0.5
0.05
UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
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™ in included in the User's Guide.
© 2000-2007 United States Environmental Protection Agency for EPI Suite™ and all component programs except BioHCWIN and KOAWIN.
start
Steve Herman - Inbo...
EPI v3.20
11:48 AM

EPI Suite

Fugacity Level III



Environmental Profile

Biodegradation

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

Atmospheric Oxidation

Model predict that this will be rapid, with ½ 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.

EPA

Chem. Rev. **2007,** *107,* 2207–2227

Designing Small Molecules for Biodegradability

R. S. Boethling,*,† Elizabeth Sommer,‡ and David DiFiore‡

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

Received September 14, 2006

Contents

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

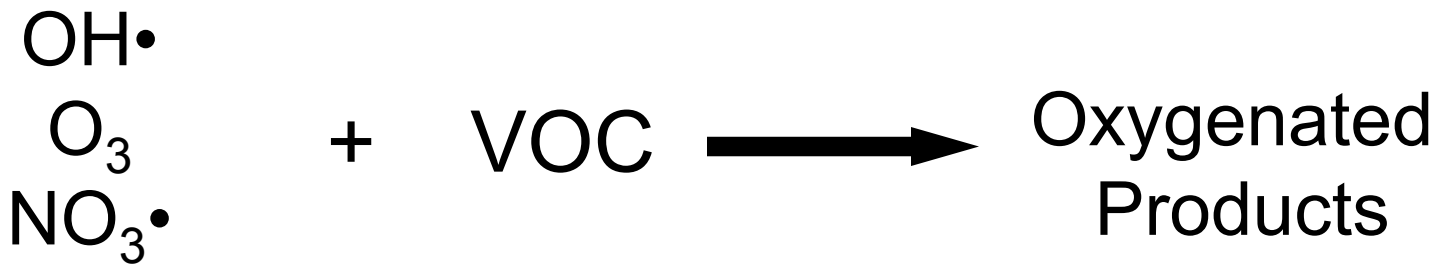
Chemistry of Indoor Environments

Ray Wells

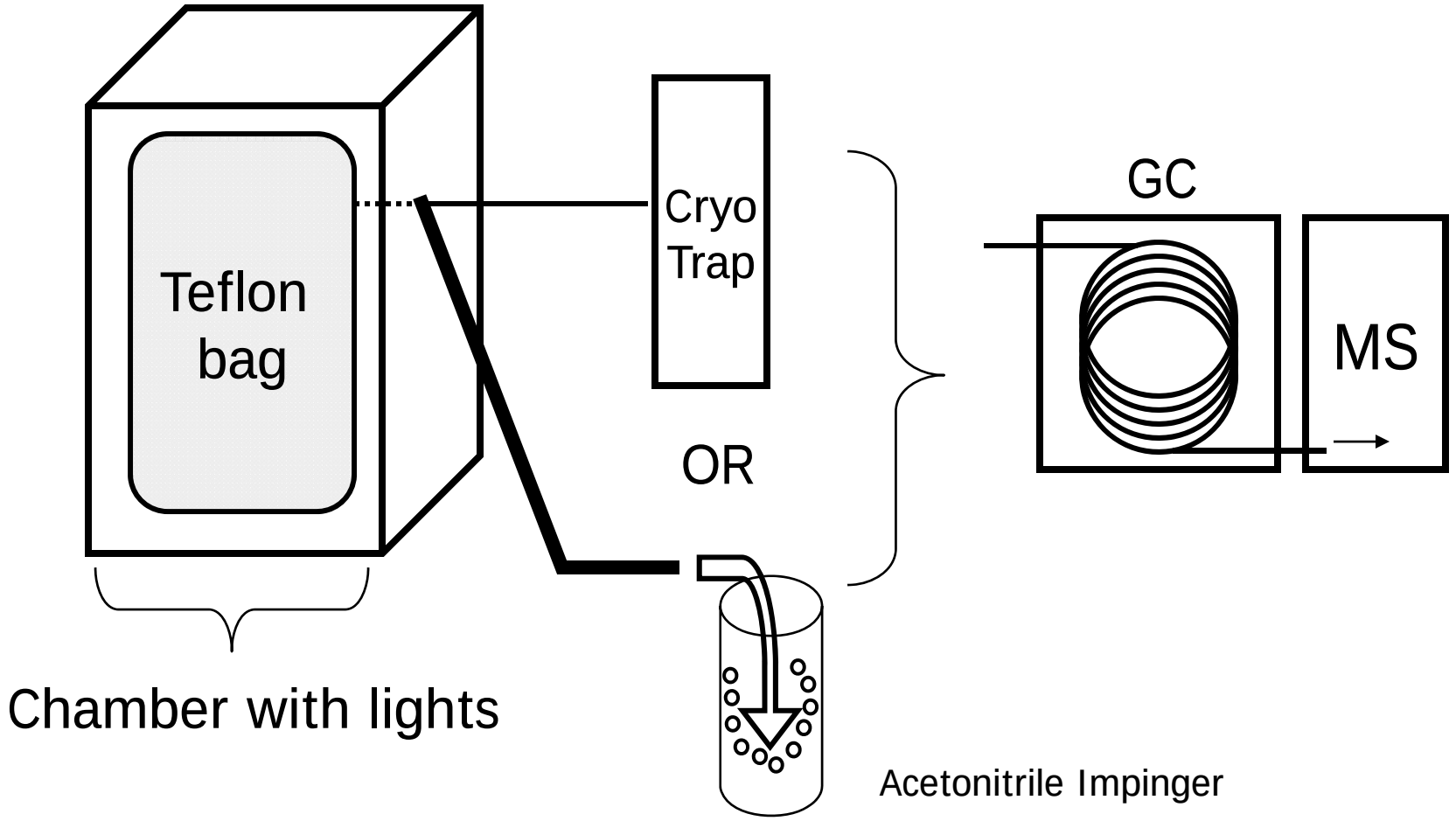
Exposure Assessment Branch
NIOSH
Morgantown, WV

Indoor Reactants

Hydroxyl Radical ($OH\bullet$)
Ozone (O_3)
Nitrate Radical ($NO_3\bullet$)



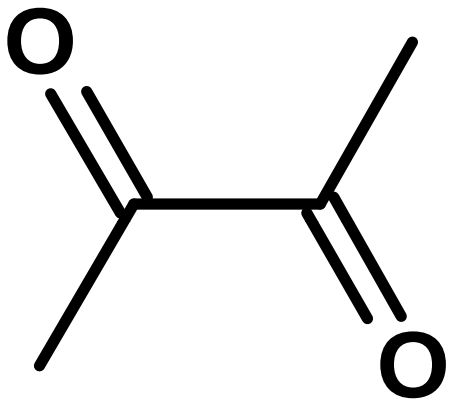
Experimental



Diacetyl

- Small oxygenated organic
- Microwave popcorn workers

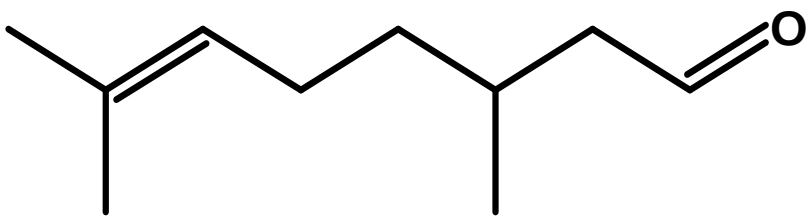
Kanwal, et al. (2006) J of Occup Env Med 48 149-157.



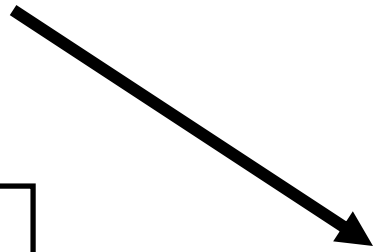
- Rat exposures – airway damage

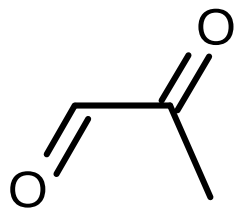
Hubbs, et al. (2002) Tox Appl Pharma 185 128-135.

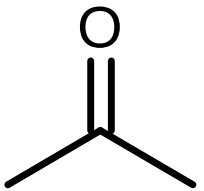
Citronellal and O_3

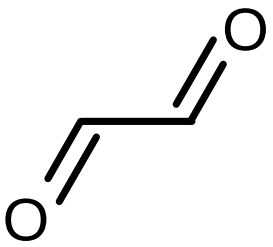


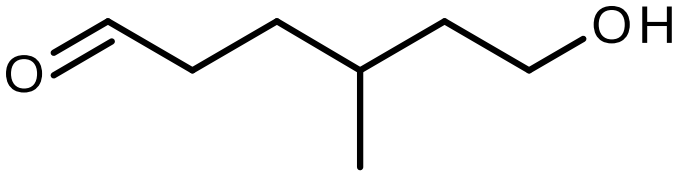
+ Reactant



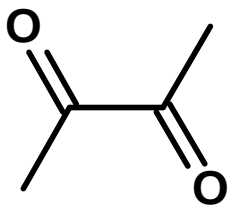






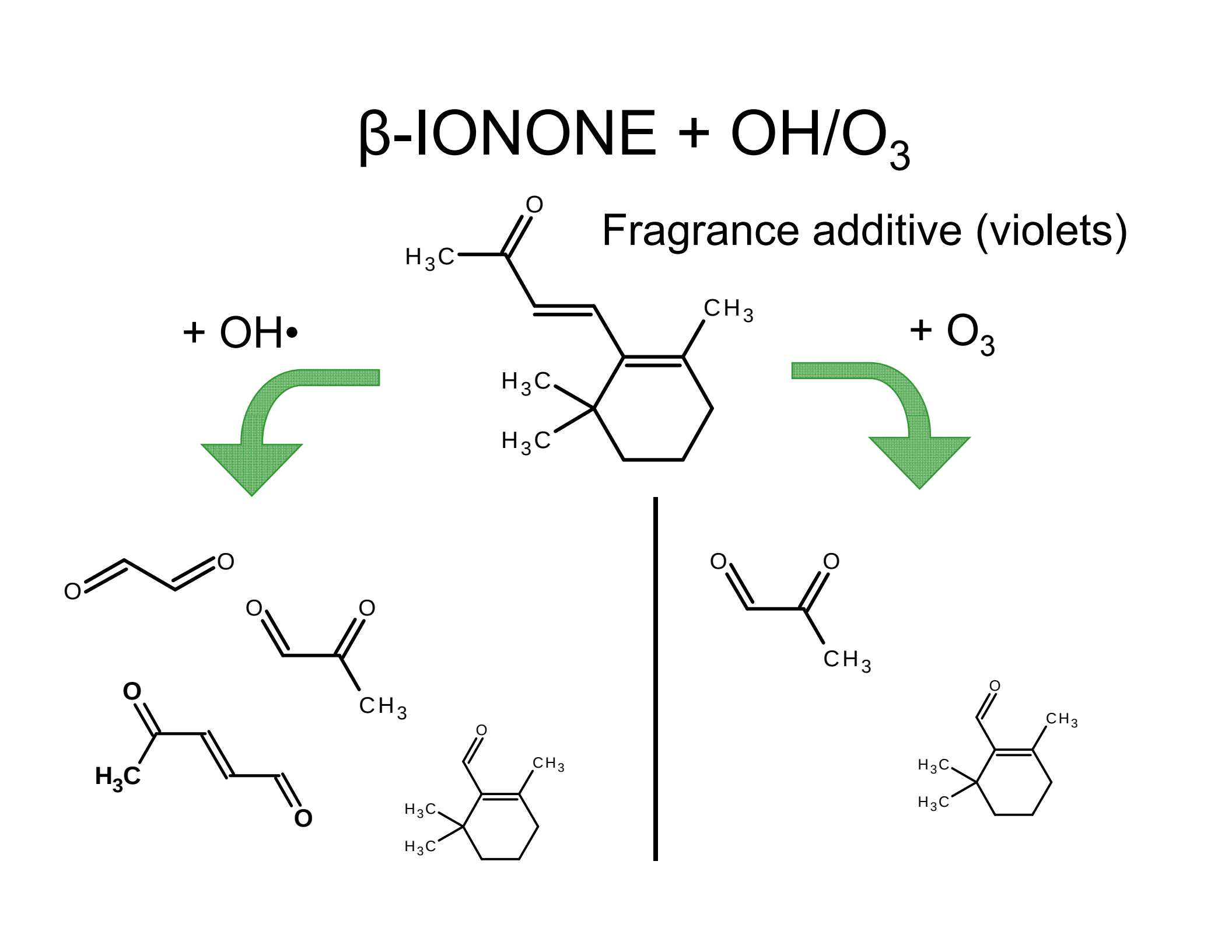


Diacetyl –

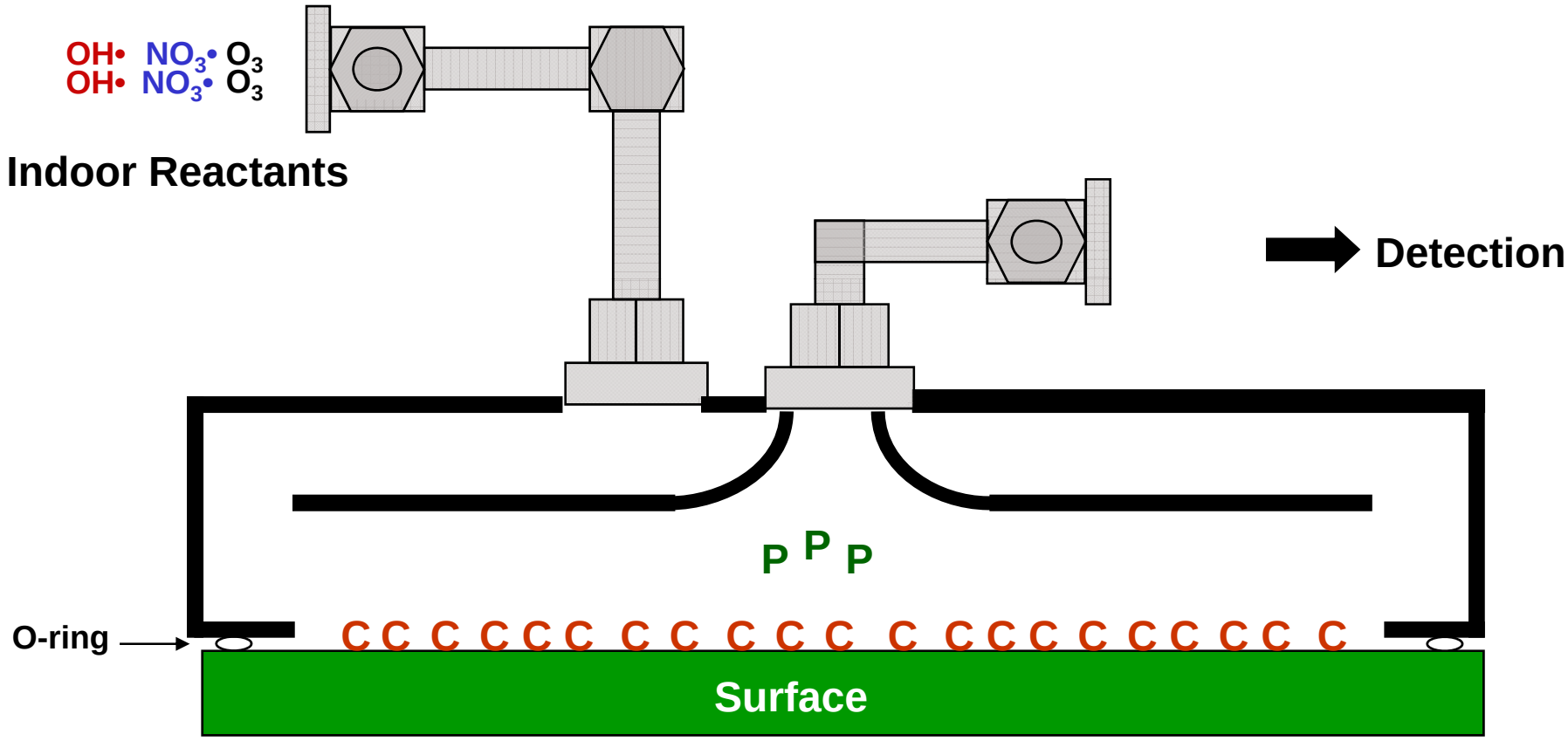


β-IONONE + OH/O_3

Fragrance additive (violets)

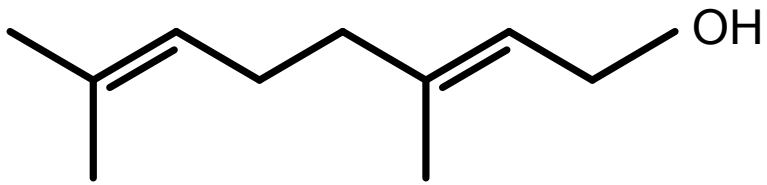


Surface Chemistry



C = chemical applied to surface

P = products formed after reaction with surface chemicals



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Atmospheric Environment 40 (2006) 726–735

ATMOSPHERIC ENVIRONMENT

www.elsevier.com/locate/atmosenv

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

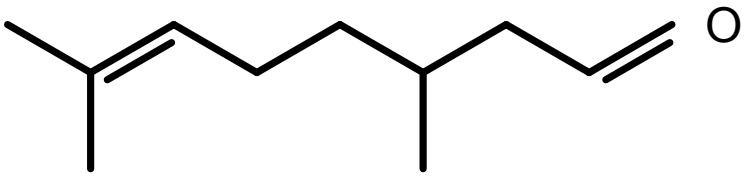
Jason E. Ham[a], Steven P. Proper[b], J.R. Wells[a,*]

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

[b]*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



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Atmospheric Environment 41 (2007) 4482–4491

ATMOSPHERIC ENVIRONMENT

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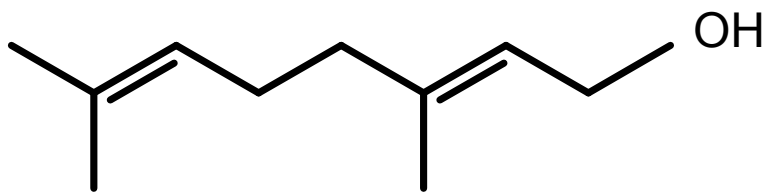
Citronellal reactions with ozone and OH radical: Rate constants and gas-phase products detected using PFBHA derivatization

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



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Atmospheric Environment 41 (2007) 1188–1199

ATMOSPHERIC ENVIRONMENT

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

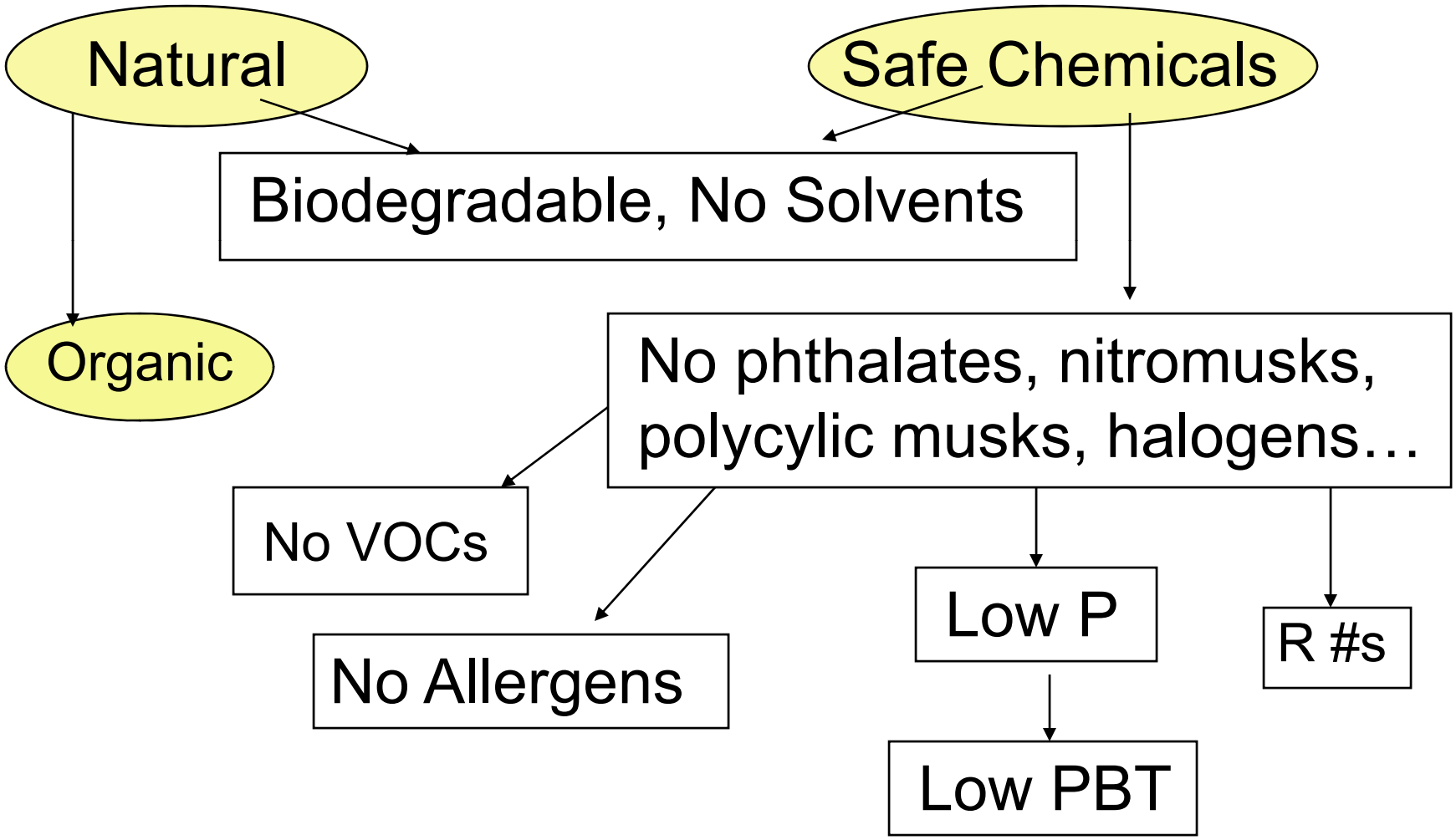
Crystal D. Forester, Jason E. Ham, J.R. Wells*

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