Improved resolution of hydrocarbon structures and constitutional isomers in complex mixtures using Gas Chromatography-Vacuum Ultraviolet-Mass Spectrometry (GC-VUV-MS)

Gabriel Isaacman\textsuperscript{a*}, Kevin R. Wilson\textsuperscript{b}, Arthur W. H. Chan\textsuperscript{a}, David R. Worton\textsuperscript{a,c}, Joel R. Kimmel\textsuperscript{d,e,f}, Theodora Nah\textsuperscript{g}, Thorsten Hohaus\textsuperscript{d}, Marc Gonin\textsuperscript{f}, Jesse H. Kroll\textsuperscript{h,i}, Doug R. Worsnop\textsuperscript{d}, and Allen H. Goldstein\textsuperscript{a,j,k}

University of California, Berkeley
Department of Environmental Science, Policy, and Management
130 Mulford Hall #3114
Berkeley, CA 94720-3114
\*gabriel.isaacman@berkeley.edu

\textsuperscript{a} Environmental Science, Policy, and Management, University of California, Berkeley, CA
\textsuperscript{b} Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA
\textsuperscript{c} Aerosol Dynamics Inc., Berkeley, CA
\textsuperscript{d} Center for Aerosol and Cloud Chemistry, Aerodyne Research, Inc., Billerica, MA
\textsuperscript{e} Cooperative Institute for Research in the Environmental Sciences and Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO
\textsuperscript{f} Tofwerk AG, Thun, Switzerland
\textsuperscript{g} Chemistry, University of California, Berkeley, CA
\textsuperscript{h} Civil and Environmental Engineering, Massachusetts Institute of Technology, Cambridge, MA
\textsuperscript{i} Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA
\textsuperscript{j} Environmental and Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, CA
\textsuperscript{k} Civil and Environmental Engineering, University of California, Berkeley, CA
This supplementary information contains the mass spectra of known compounds using vacuum ultraviolet (VUV) ionization at transfer temperatures of 150 °C (38 compounds) and 275 °C (84 compounds). Parent ion is shown in bold (not shown for chlorinated compounds because the prevalence of both $^{35}$Cl and $^{37}$Cl leads to multiple "parent" ions). Mass spectra using electron impact (EI) ionization for all reported compounds are available online from the NIST WebBook (reference provided in manuscript).

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S.1. Spectra at a transfer temperature of 150 °C

S.1.1. Normal alkanes

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**tetradecane**

Ion abundance (arb. units)

Ion mass-to-charge, m/Q (Th)

198

VUV: 150 °C, 10.5 eV

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**pentadecane**

Ion abundance (arb. units)

Ion mass-to-charge, m/Q (Th)

212

VUV: 150 °C, 10.5 eV
hexadecane

Ion mass-to-charge, m/Q (Th)

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV

heptadecane

Ion mass-to-charge, m/Q (Th)

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV

octadecane

Ion mass-to-charge, m/Q (Th)

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV
S.1.2. Branched aliphatic hydrocarbons

**Phytane**
- VUV: 150 °C, 10.5 eV
- Ion mass-to-charge, m/Q (Th)
- Ion abundance (arb. units)

- Ion masses: 126, 183, 282

**Pristane**
- VUV: 150 °C, 10.5 eV
- Ion mass-to-charge, m/Q (Th)
- Ion abundance (arb. units)

- Ion masses: 112, 154, 183, 268
S.1.3. Acids

3,4-dimethoxybenzoic acid & homovanillic acid (coelution) VUV: 150 °C, 10.5 eV

4-methylphthalic acid VUV: 150 °C, 10.5 eV
isopimaric acid

hexadecanoic acid

octadecanoic acid

VUV: 150 °C, 10.5 eV

Ion abundance (arb. units)

Ion mass-to-charge, m/Q (Th)
cis-5,8,11,14,17-eicosapentaenoic acid

VUV: 150 °C, 10.5 eV

Ion abundance (arb. units)

Ion mass-to-charge, m/Q (Th)

108
166
148
284
302
S.1.4. Aromatics and oxygenated polycyclic aromatic hydrocarbons

**Graph of dodecyl benzene**

- Ion mass-to-charge, m/Q (Th): 246
- Ion abundance (arb. units): 92
- Conditions: VUV: 150 °C, 10.5 eV

**Graph of phenanthrene**

- Ion mass-to-charge, m/Q (Th): 178
- Ion abundance (arb. units)
- Conditions: VUV: 150 °C, 10.5 eV
chrysene

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV

228

4,4-dimethoxybenzophenone

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV

242

9H-fluoren-9-one

Ion abundance (arb. units)

VUV: 150 °C, 10.5 eV

180
S.1.5. Other oxygenated compounds (ketones, esters, aldehydes)

Hexadecanoic methyl ester

Octadecanoic methyl ester

VUV: 150 °C, 10.5 eV
2-pentadecanone

VUV: 150 °C, 10.5 eV

Ion abundance (arb. units)

ion mass-to-charge, m/Q (Th)

2-octadecanone

VUV: 150 °C, 10.5 eV

Ion abundance (arb. units)

ion mass-to-charge, m/Q (Th)

γ-dodecalactone

VUV: 150 °C, 10.5 eV

Ion abundance (arb. units)

ion mass-to-charge, m/Q (Th)
S.2. Spectra at a transfer temperature of 275 °C
S.2.1. Normal alkanes

- Tetradecane
  - Ion mass-to-charge, m/Q (Th)
  - Ion abundance (arb. units)
  - VUV: 275 °C, 10.5 eV

- Pentadecane
  - Ion mass-to-charge, m/Q (Th)
  - Ion abundance (arb. units)
  - VUV: 275 °C, 10.5 eV
S.2.2. Branched aliphatic hydrocarbons
S.2.3. Hopanes and steranes

**17α(H)-22,29,30-trisnorhopane**

VUV: 275 °C, 10.5 eV

**17α(H),21β(H)-30-norhopane**

VUV: 275 °C, 10.5 eV
S.2.4. Acids

3,4-dimethoxybenzoic acid & homovanillic acid (coelution)

VUV: 275 °C, 10.5 eV

4-methylphthalic acid

VUV: 275 °C, 10.5 eV
S.2.5. Aromatics and oxygenated polycyclic aromatic hydrocarbons

![Graph of dodecyl benzene](image)

- **VUV: 275 °C, 10.5 eV**
  - Ion abundance (arb. units)
  - Ion mass-to-charge, m/Q (Th)
  - Ion abundance (arb. units)
  - Ion mass-to-charge, m/Q (Th)

- **Phenanthrene**
  - 178

- **Dodecyl benzene**
  - 246

- **VUV: 275 °C, 10.5 eV**
  - Ion abundance (arb. units)
  - Ion mass-to-charge, m/Q (Th)
9H-fluoren-9-one

VUV: 275 °C, 10.5 eV

9,10-anthracenedione

VUV: 275 °C, 10.5 eV

Xanthone

VUV: 275 °C, 10.5 eV
S.2.6. Phthalates and other oxygenated aromatics

![Mass spectra of dimethyl phthalate and diethyl phthalate](image)

**Dimethyl Phthalate**: VUV: 275 °C, 10.5 eV

**Diethyl Phthalate**: VUV: 275 °C, 10.5 eV
S.2.7. Nitrogenated aromatics
4,6-dinitro-2-methyl phenol

VUV: 275 °C, 10.5 eV

Ion abundance (arb. units)

Ion mass-to-charge, m/Q (Th)
S.2.8. Chlorinated aromatics
S.2.9. Oxygenated aliphatic compounds (ketones, esters, aldehydes)
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