ANALYSIS OF THE
ORGANIC MASS SPECTRA

Typical Ambient Mass Spectrum

INORGANICS/AIR:
Air m/z’s: 14(N⁺), 28(N₂⁺), 32(O₂⁺), 40 (CO⁺)

Water m/z’s: fragment of 18 (H₂O⁺)
Nitrate m/z’s: 30 (NO⁻), 46 (NO₂⁻)
Sulphate m/z’s: 48 (SO⁺), 64 (SO₂⁺), 80 (SO₃⁺), 81 (SO₃⁺)
Ammonium m/z’s: fragments of 15 (NH, 16 (NH₂⁺),
17 (NH₃⁺)
Chloride m/z’s: fragments of 36 (H₃5Cl, 38 (H₃7Cl)

ORGANICS:
No separation of individual species prior to vaporization & ionization
Overlapping patterns of multiple molecules.
Field Spectra:

1) Look at Correlations in Time and Size of Fragments to Identify those that may belong to same parent

2) Look at correlations in time between organic fragments and Gas phase measurements

“Typical” aerosol mass spectra

Aerosol composition can be classified from mass spectrum
Ion Series in Mass Spectra

- CH₂ Ion Series**: “Picket Fence” like spectra in which groups of peaks have 14 amu separation.

- Masses at which peaks appear are characteristic of R backbone. Series with different R’s are classified according to their \( \Delta \) value

\[
\Delta = \text{Peak mass} - 14n + 1
\]

*“Interpretation of Mass Spectra” by McLafferty F.W. and Turecek, F.

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Diesel Aerosol Composition

Main Chemical Compounds in Diesel and Lubricant Oil:

- n-alkanes
- branched alkanes
- cyloalkyl species
“Typical” aerosol mass spectra

\[ 44 \text{ (CO}_2^+ \) \]

\[ \text{CO}_2^+ \text{ is marker for oxygenated organic} \]

“hydrocarbon”

\[ e^- \]

\[ \text{C}_n\text{H}_m \rightarrow \text{C}_n'\text{H}_m'^+ \]

“oxygenated”

\[ e^- \]

\[ \text{CnHmOy} \rightarrow \text{CO}_2^+ \text{, H}_3\text{C}_2\text{O}^+ \text{, HCO}_2^+ \text{, Cn'Hm'}^+ \]

\[ 44 \quad 43 \quad 45 \quad 55, 57, \ldots \]

Application of Delta Analysis to Field Data:

( NYC Supersite - Frank Drewnick)

Traffic Related Particles

Composition - Organic Particles

Photochemical Particles

Data
Examples of Mass Spectra seen by various AMS Users……

What we are looking for is common features among these spectra that may be useful in determining the relative importance of various organic groups in the organic Mass Spectra.

Combustion Sources
Urban Mixes
Photochemical Time Periods
Rural/Biogenic/Marine Environments
Note: even though this was supposed to be a rural site, it had quite a bit of urban influence from nearby towns.
Lab Experiments
ARI metallic acid

ARI diesel fuel

Lognormal Fit
median = 3.42
width = 0.41
Acknowledgements to the AMS Users for sharing their Mass Spectra with us for this compilation!!!