

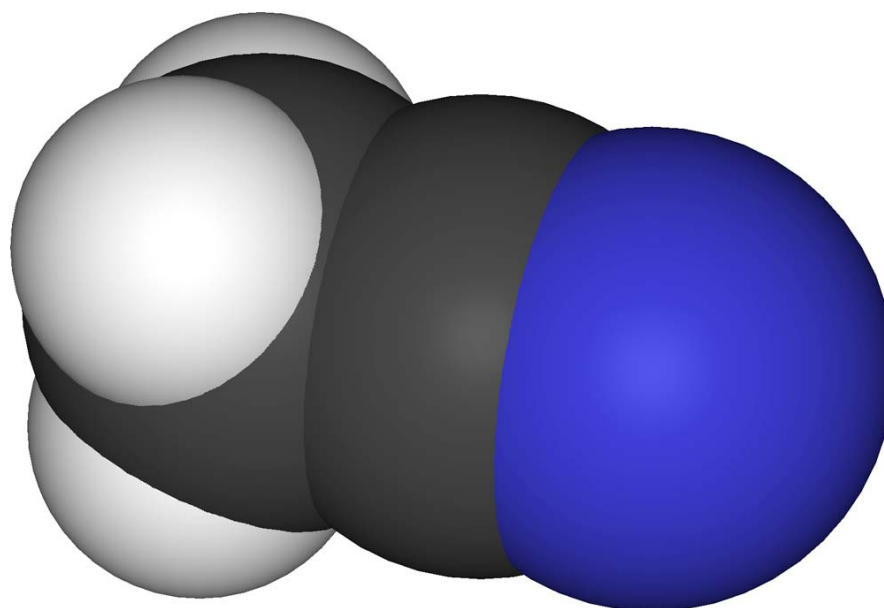
# **CoSMoS 2009**

Impact of the Acetonitrile Crisis on  
Separation Technology and  
Chromatography Labs

**PTI**

# **Acetonitrile**

**Simple Molecule – Complex Problem**



# **PTI** Purification Technologies Incorporated

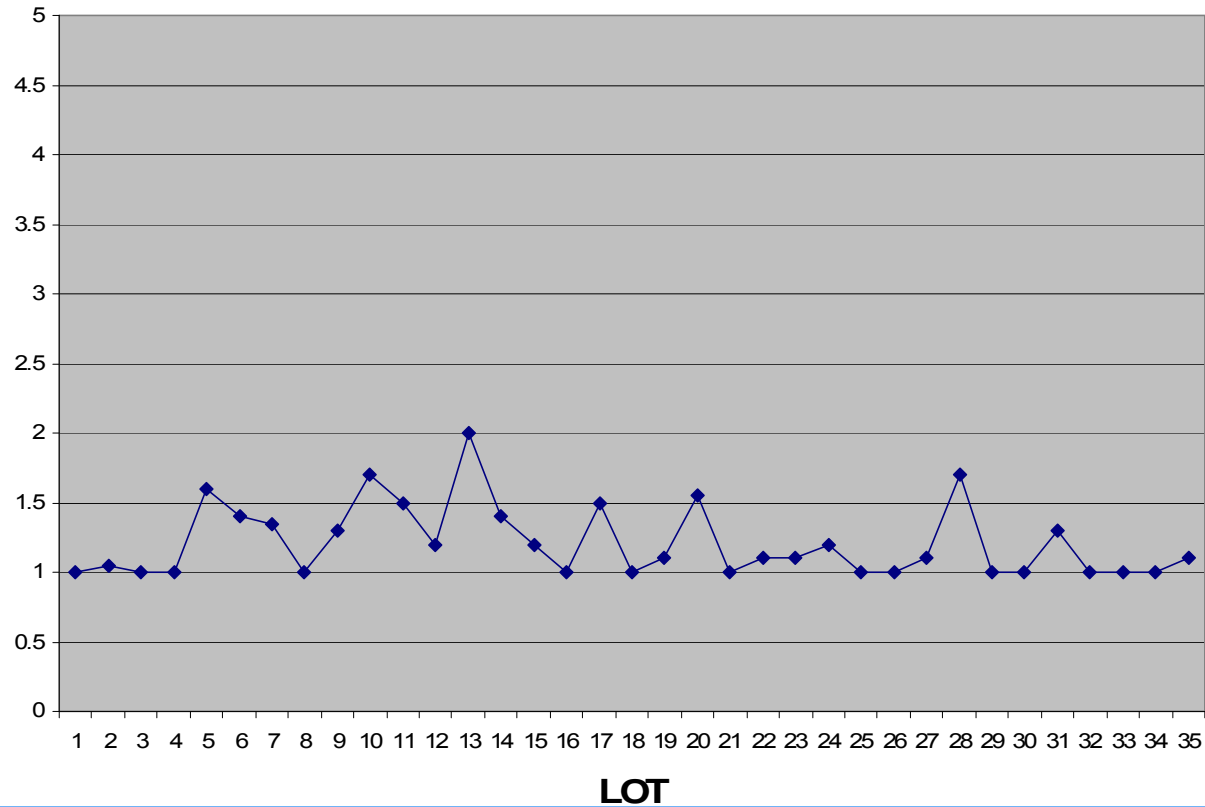




# Largest Bulk Supplier of Ultra Low Water – HPLC Gradient Quality Acetonitrile

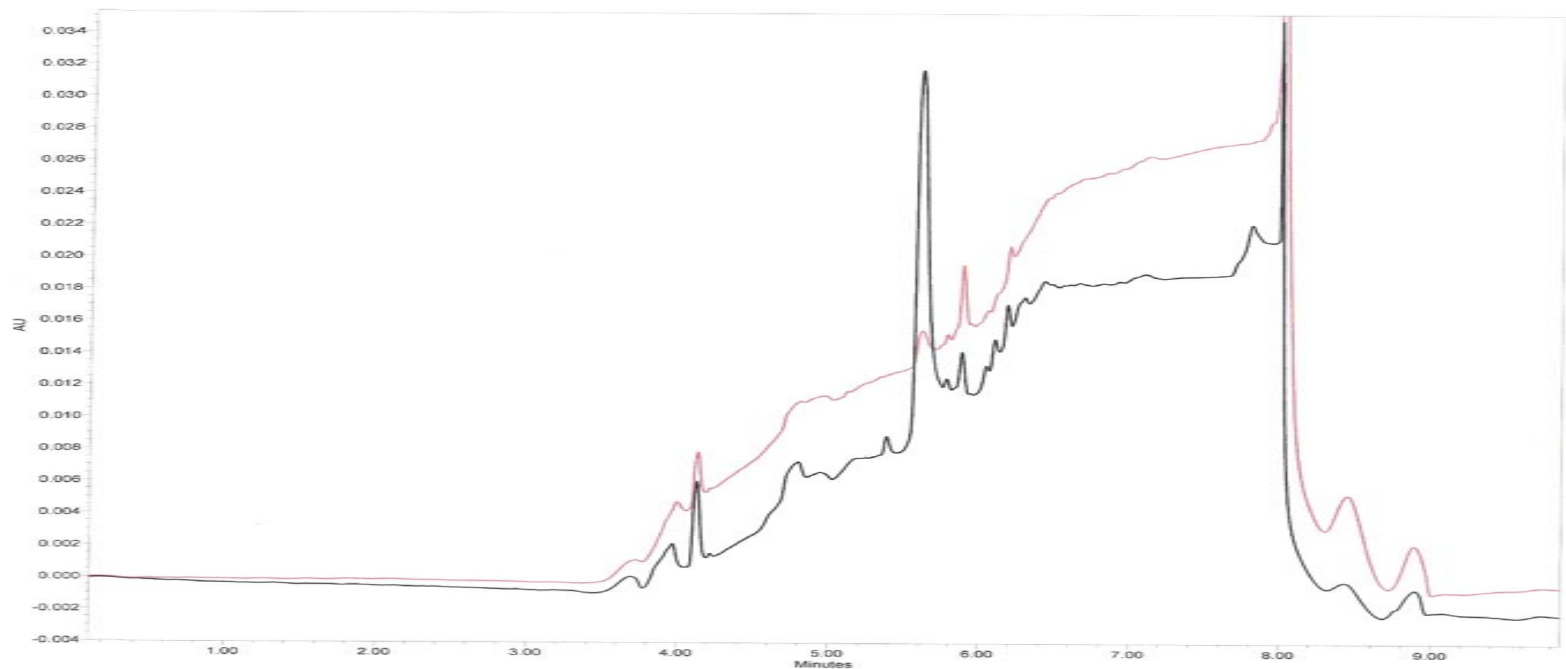


## Actual Water Content Finished Tankers



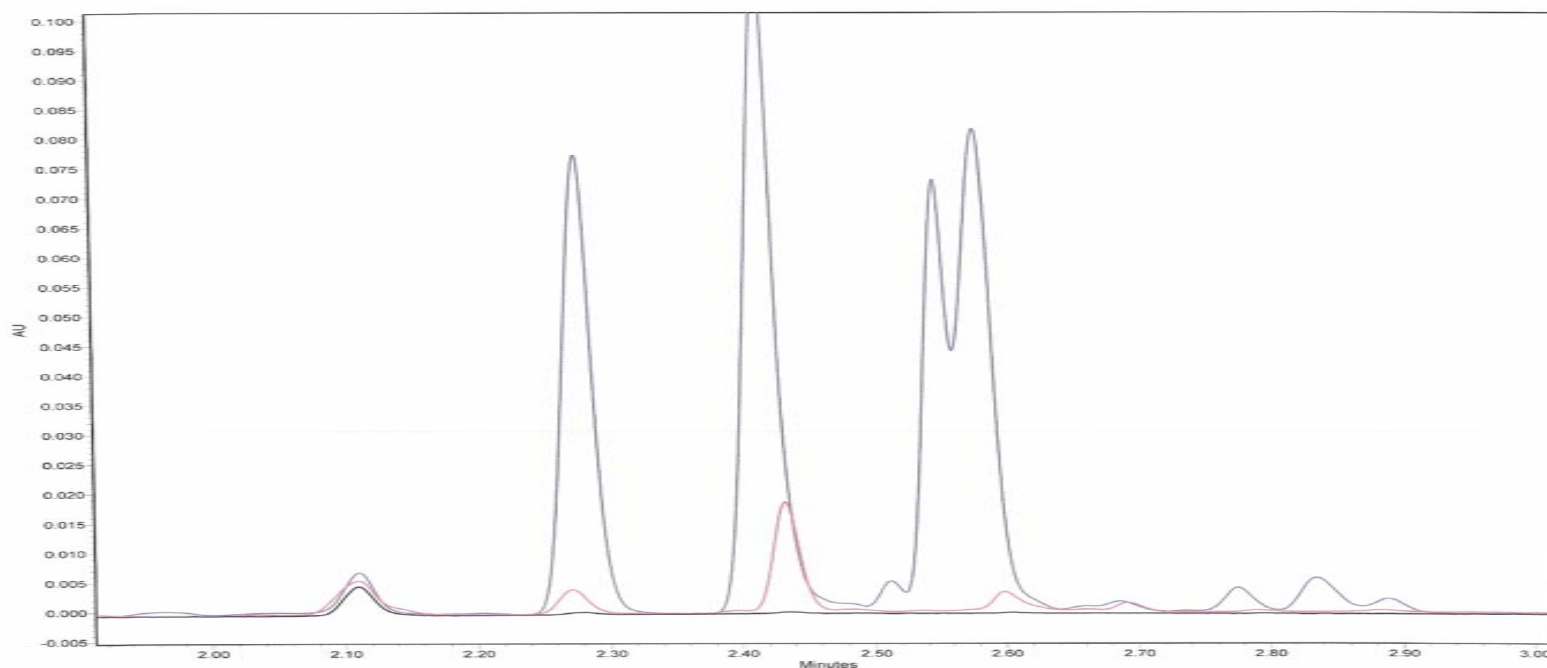


# Part per Billion Purity UPLC Gradient vs 10 ppb Toluene





# Part per Billion Purity Trace Carbonyls vs 20 ppb Acetone



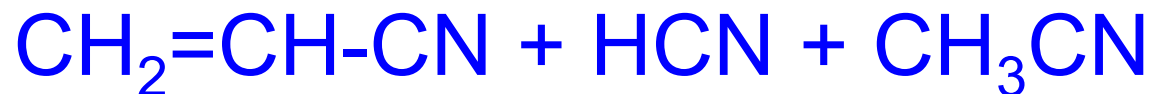


# Acrylonitrile Synthesis

Propylene Ammoxidation – Sohio Process



↓ Catalyst



Major Commercial Products

# **PTI** Purification Technologies Incorporated

**Co-Product**

**Commercial**

**HPLC/Low Water**

**Acetonitrile**

**Acetonitrile**

**Acetonitrile**

60% - 80% Pure

→

99.9% Pure

→

Low Trace Impurities

↓

Not Recovered

↓

Used in Pharmaceutical  
or

Organic Synthesis

↓

HPLC Analysis

DNA Synthesis

## **Co-Product Acetonitrile (60 – 80%) Major Impurities**

- Water (15 – 25%)
- Acetone
- Acrolein
- Acrylonitrile
- Allyl Alcohol
- Cis/trans Crotononitrile
- Hydrogen Cyanide
- Methanol
- Methacrylonitrile
- Oxazole
- Propionitrile
- Toluene (trace)
- Others

## **Crude Co-Product Acetonitrile to 99.95% Purification Methods**

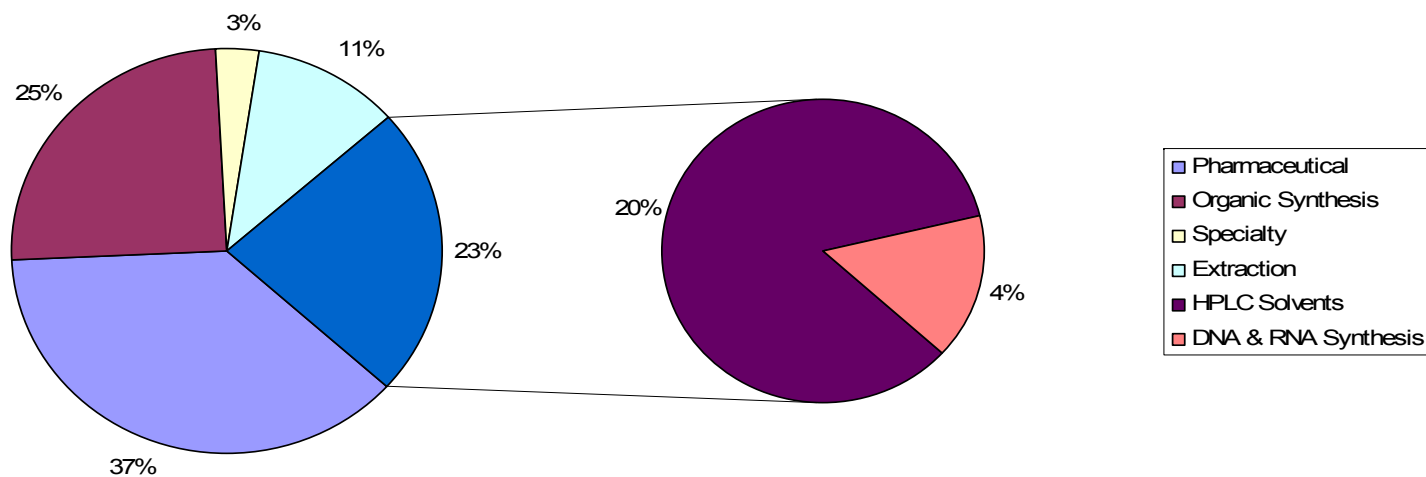
- Multi Steps: Chemical Treatment & Distillation
- Chemical Treatment:
  - Caustic (water, HCN, acrolein, acrylonitrile)
  - Acid (oxazole, water)
  - Oxidation (acrylonitrile, oxazole, allyl alcohol)
- Distillation:
  - Entrainer (water)
  - Light ends removal
  - Heavies
  - Pressure swing distillation



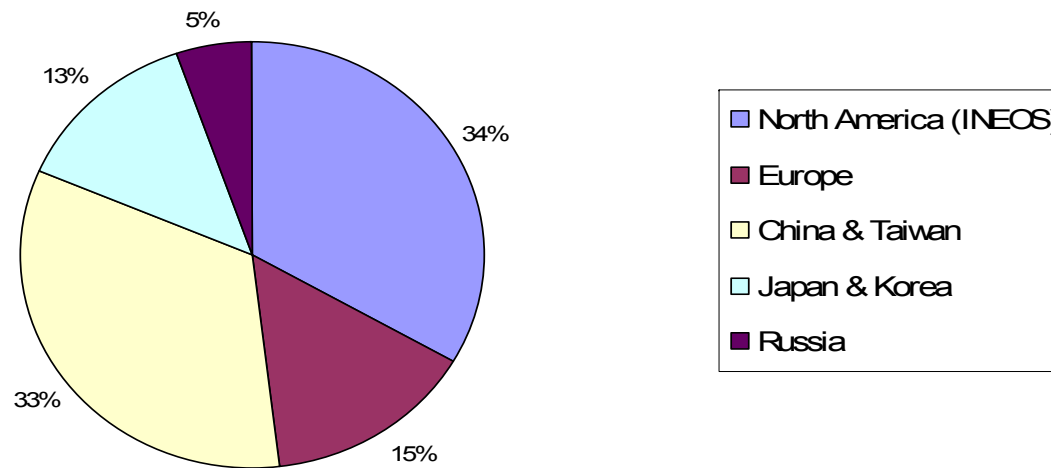
## **99.95% Acetonitrile to HPLC Common Purification Methods**

- Multi Steps: Chemical Treatment & Distillation or Other Method
- Chemical Treatment:
  - Oxidation (trace UV absorbing impurities)
- Distillation:
  - Light ends removal
  - Residue and Higher Boiling Impurities

## Acetonitrile Useage by Application



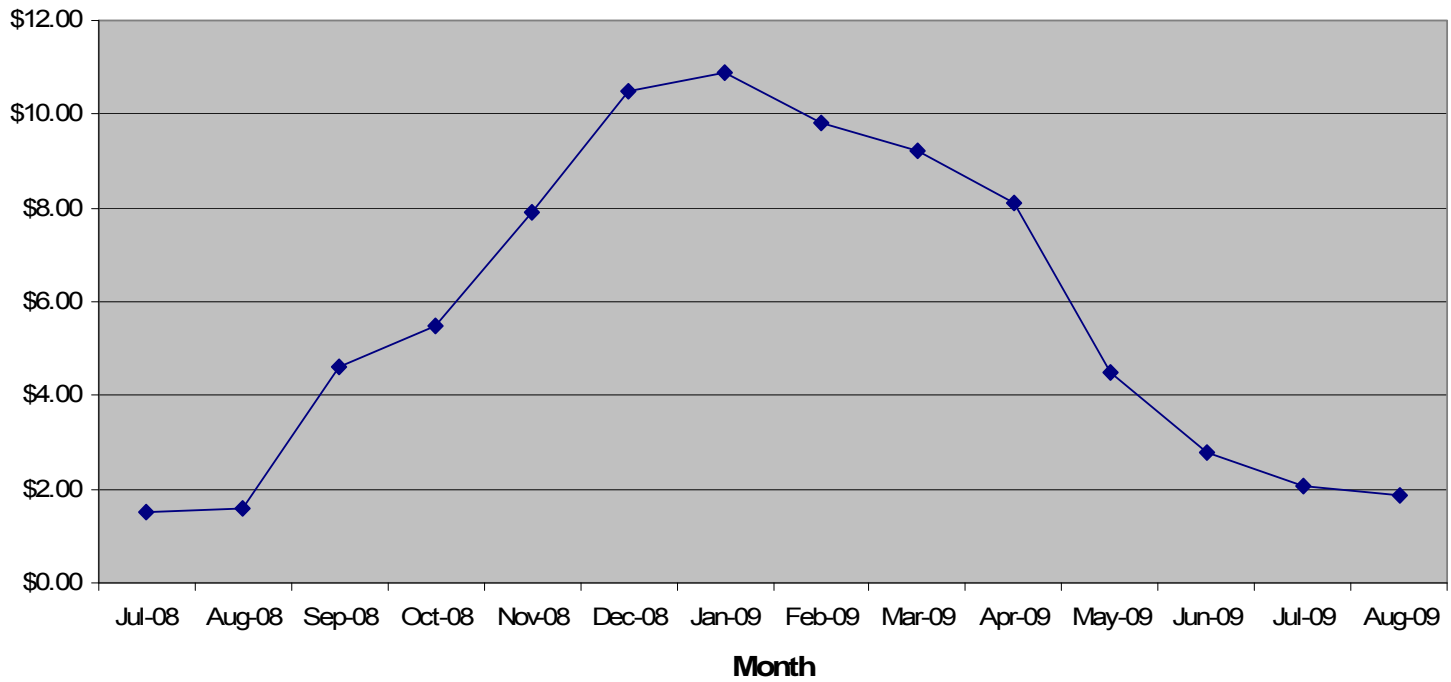
## Acetonitrile Worldwide Supply



## United States Acrylonitrile Plants

- INEOS – Recovers and Markets Acetonitrile
  - Green Lake, TX
  - Lima, OH
- Lucite – Beaumont, TX
  - Third party processors of acetonitrile
- Solutia – Chocolate Bayou, TX
  - Do not recover Acetonitrile, HCN focus
- Cytec Co-Product Stream
  - Previously Not Recovering Acetonitrile
  - 12 million lbs/yr New to Market

**Acetonitrile Supply  
Bulk Shortage Prices  
\$/Lb**



## Future Status of Acetonitrile Market?

- **Strength of Demand**
  - Pharmaceutical Manufacturing (Multi-million pound usage)
    - India and China
    - Europe
  - Biotechnology Applications
    - Peptides
    - Oligonucleotides
  - Specialty Chemicals
  - HPLC Applications
  - Other Applications (electronic)
- **Supply Linked to Acrylonitrile**
  - Demand for Acrylonitrile (acrylic fibers, acrylic plastics, polyacrylamide)
  - Impact of Alcohol Injection
- **Other Potential Sources of Supply**
  - Recycling: technical, regulatory and business hurdles

**Other Potential Sources of Supply:  
Direct Synthesis of Acetonitrile?**

- A.  $\text{CH}_3\text{OH} + \text{HCN} \rightarrow \text{CH}_3\text{CN} + \text{H}_2\text{O}$
- B.  $\text{CH}_3\text{COOH} + \text{NH}_3 \rightarrow \text{CH}_3\text{CONH}_2 + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{CN} + \text{H}_2\text{O}$
- C.  $\text{CO} + \text{NH}_3 + \text{H}_2 \rightarrow \text{CH}_3\text{CN} + \text{H}_2\text{O}$
- D.  $\text{CH}_3\text{CH}_2\text{OH} + \text{NH}_3 \rightarrow \text{CH}_3\text{CN} + \text{H}_2\text{O}$
- E.  $\text{CH}_3\text{CH}_3 + \text{NH}_3 \rightarrow \text{CH}_3\text{CN} + \text{H}_2$

**Common Issues for Synthesis:**

Catalyst and process development

Process safety

Investment cost

Unit cost (synthesis and purification)