

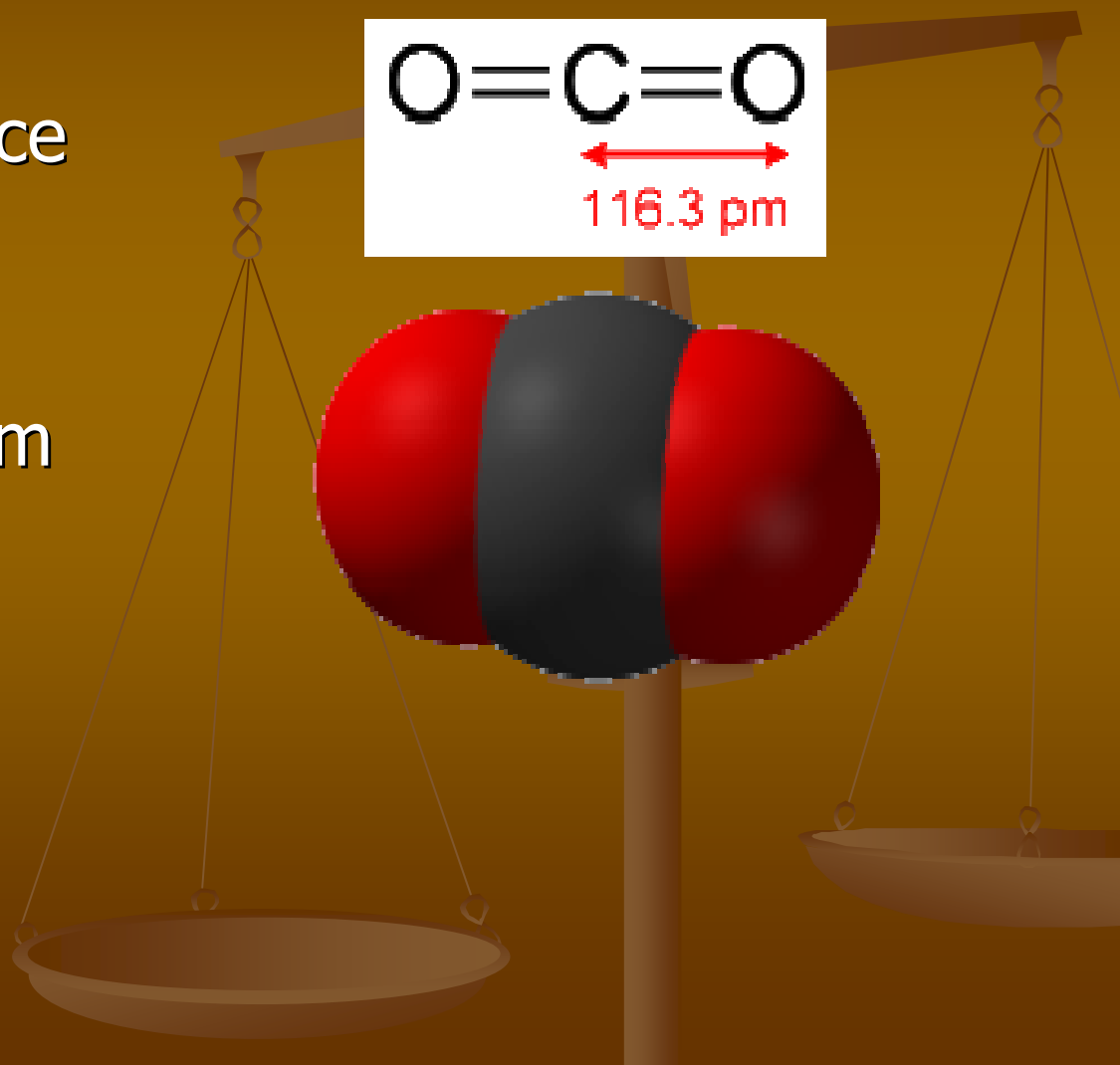
CO₂: An Alternate Solvent

By: Greg Essligner



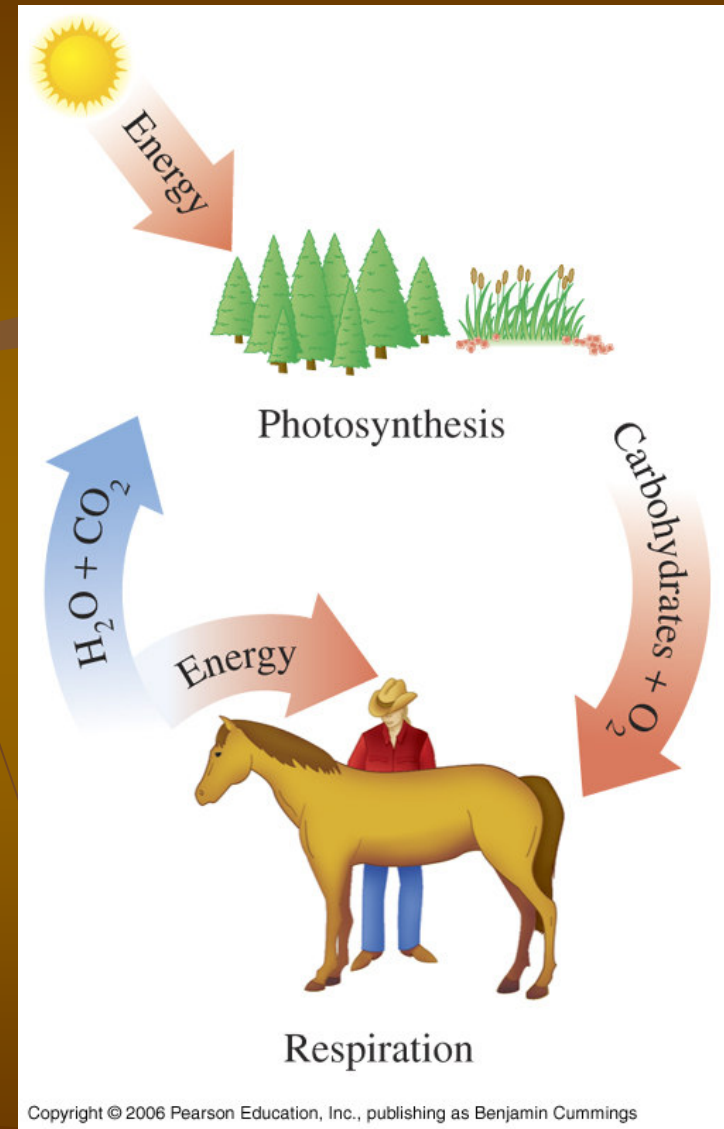
Carbon Dioxide

- CO_2
- Solid phase: Dry Ice
- 44.0095(14)g/mol
- M.P. -57°C (when pressurized 5.1 atm or higher)
- B.P. -78°C (sublimation)
- No Dipole



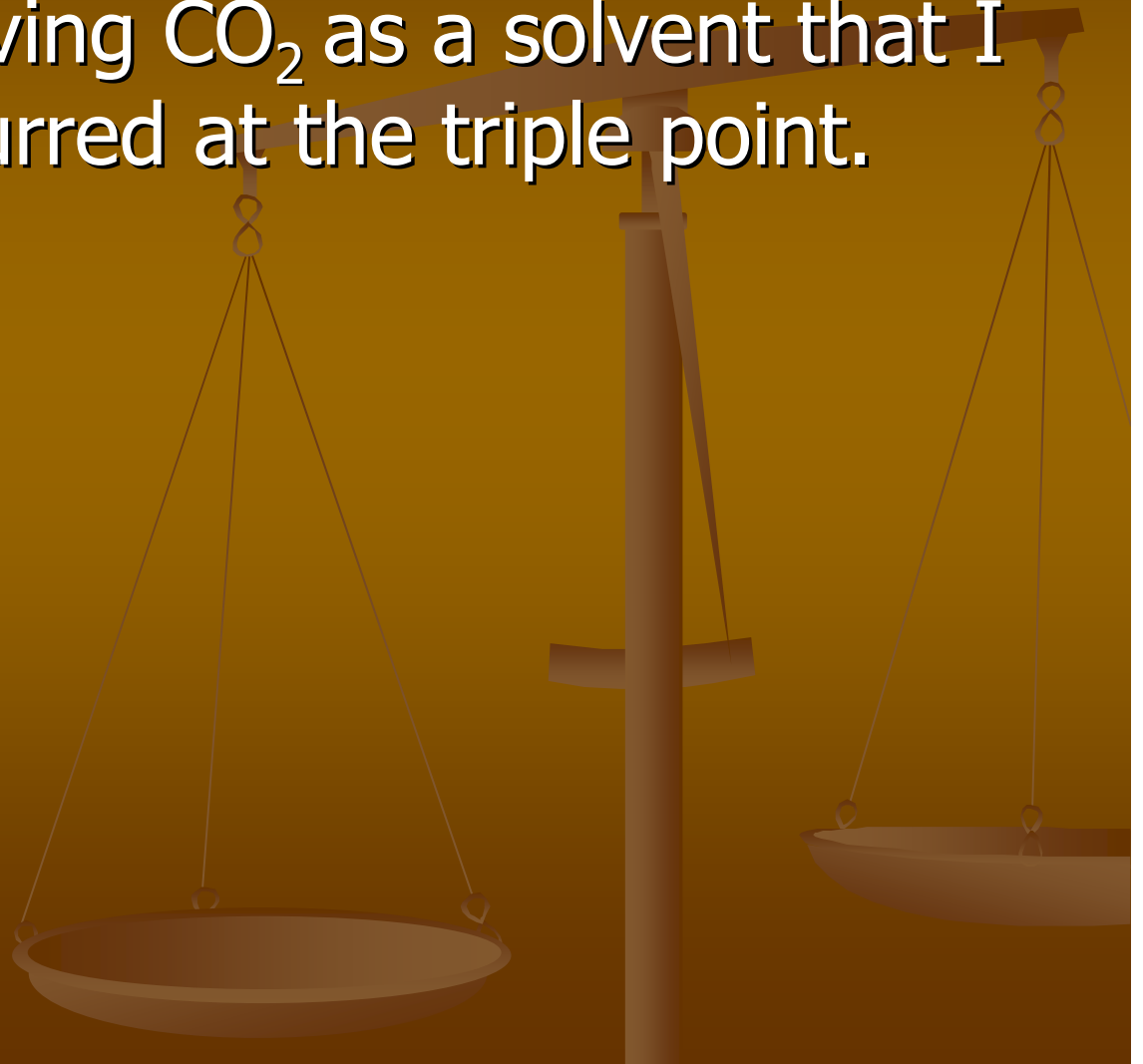
Common Uses

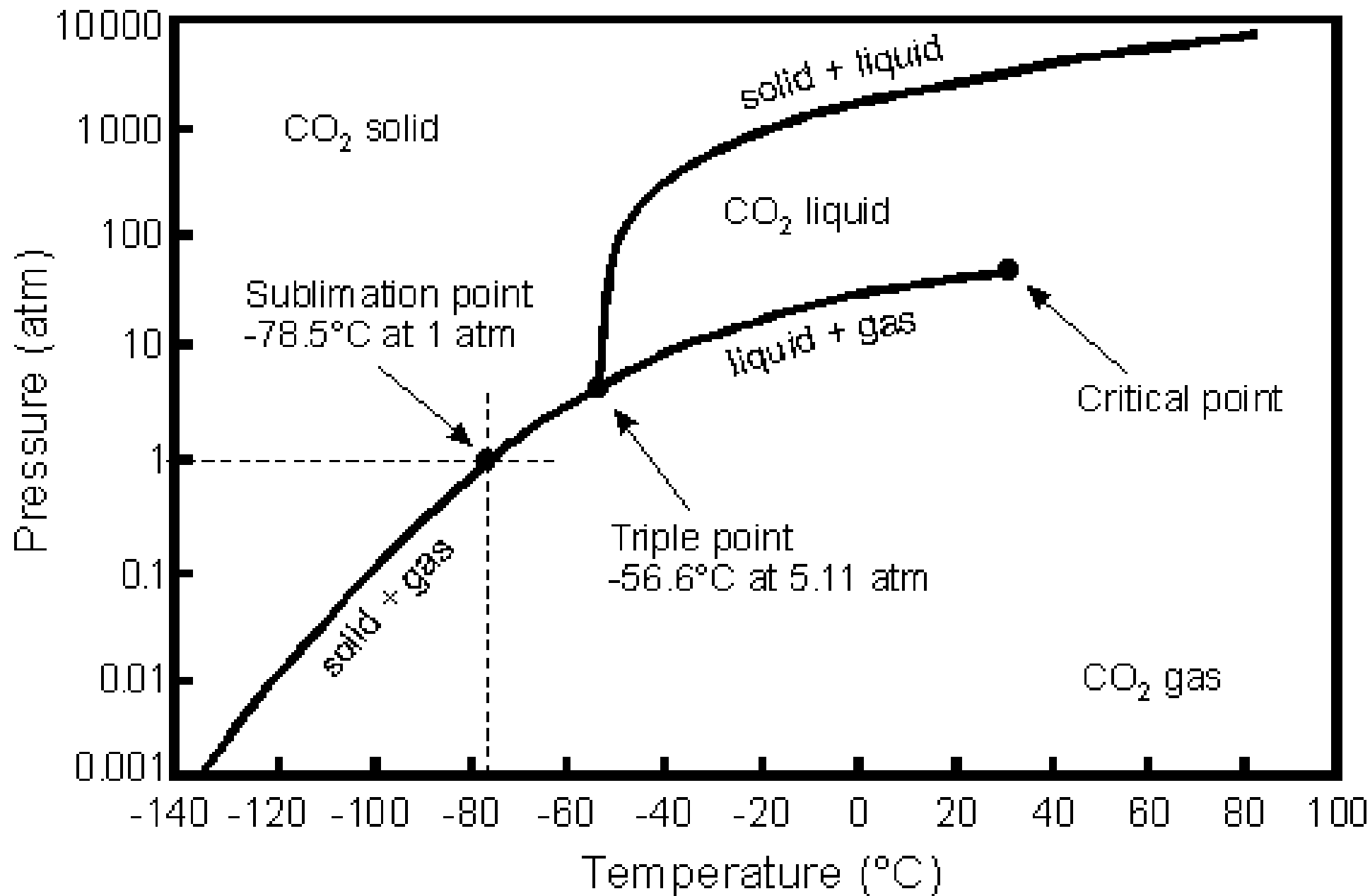
- Carbon Cycle
 - Photosynthesis
- Fog machines



Phase Diagram

- Chemistry involving CO_2 as a solvent that I researched occurred at the triple point.

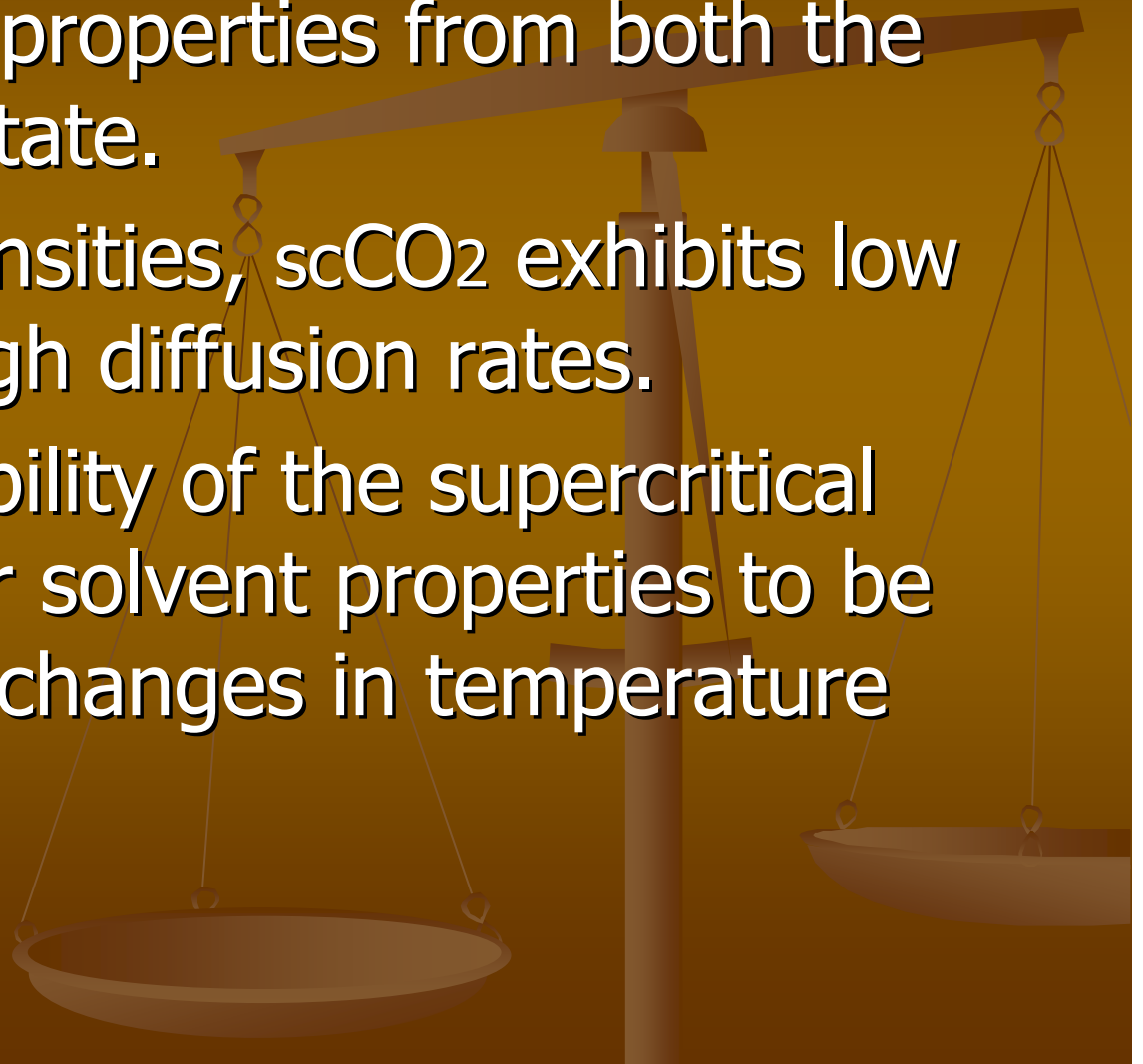




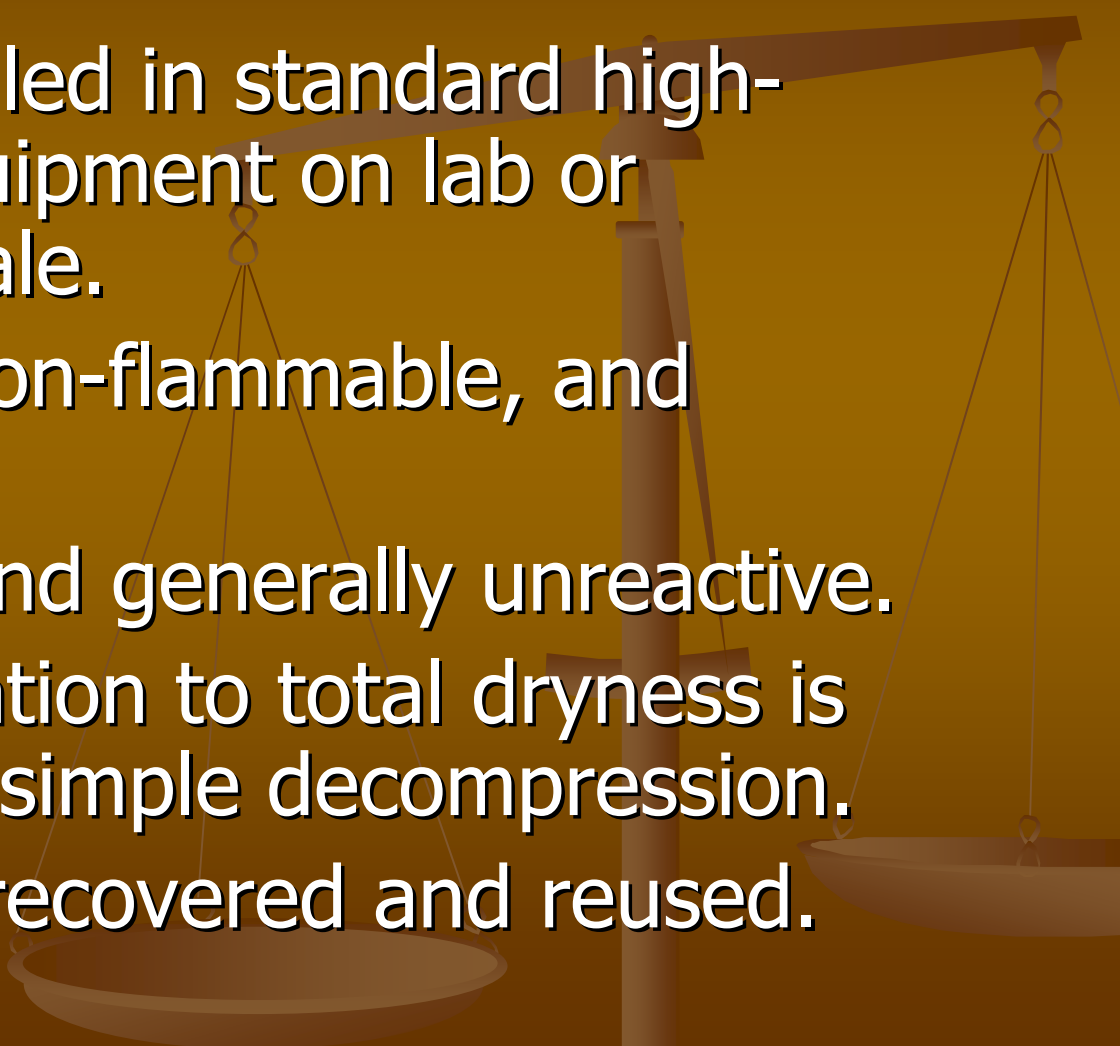
Pressure-Temperature phase diagram for CO₂.

Properties of $scCO_2$

- Combination of properties from both the liquid and gas state.
- At liquid-like densities, $scCO_2$ exhibits low viscosity and high diffusion rates.
- High compressibility of the supercritical phase allows for solvent properties to be varied by small changes in temperature and pressure.

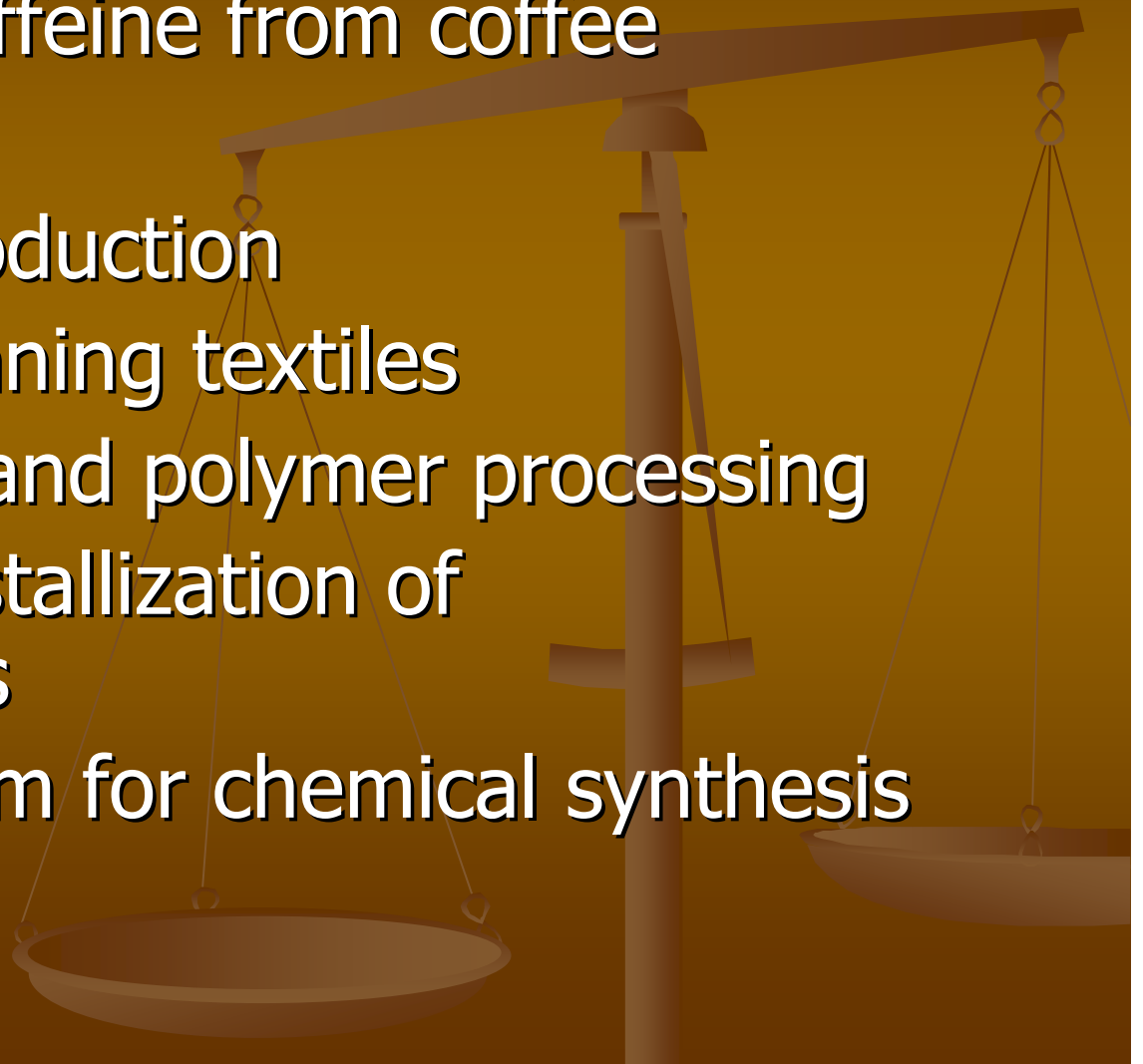


Properties of scCO₂

- Can be handled in standard high-pressure equipment on lab or industrial scale.
 - Non-toxic, non-flammable, and inexpensive.
 - Non-protic and generally unreactive.
 - Product isolation to total dryness is achieved by simple decompression.
 - CO₂ can be recovered and reused.
- 

Current / Future Uses of $scCO_2$

- Extraction of caffeine from coffee
- Dry cleaning
- Hops aroma production
- Dyeing and cleaning textiles
- Polymerization and polymer processing
- Purification/crystallization of pharmaceuticals
- Reaction medium for chemical synthesis



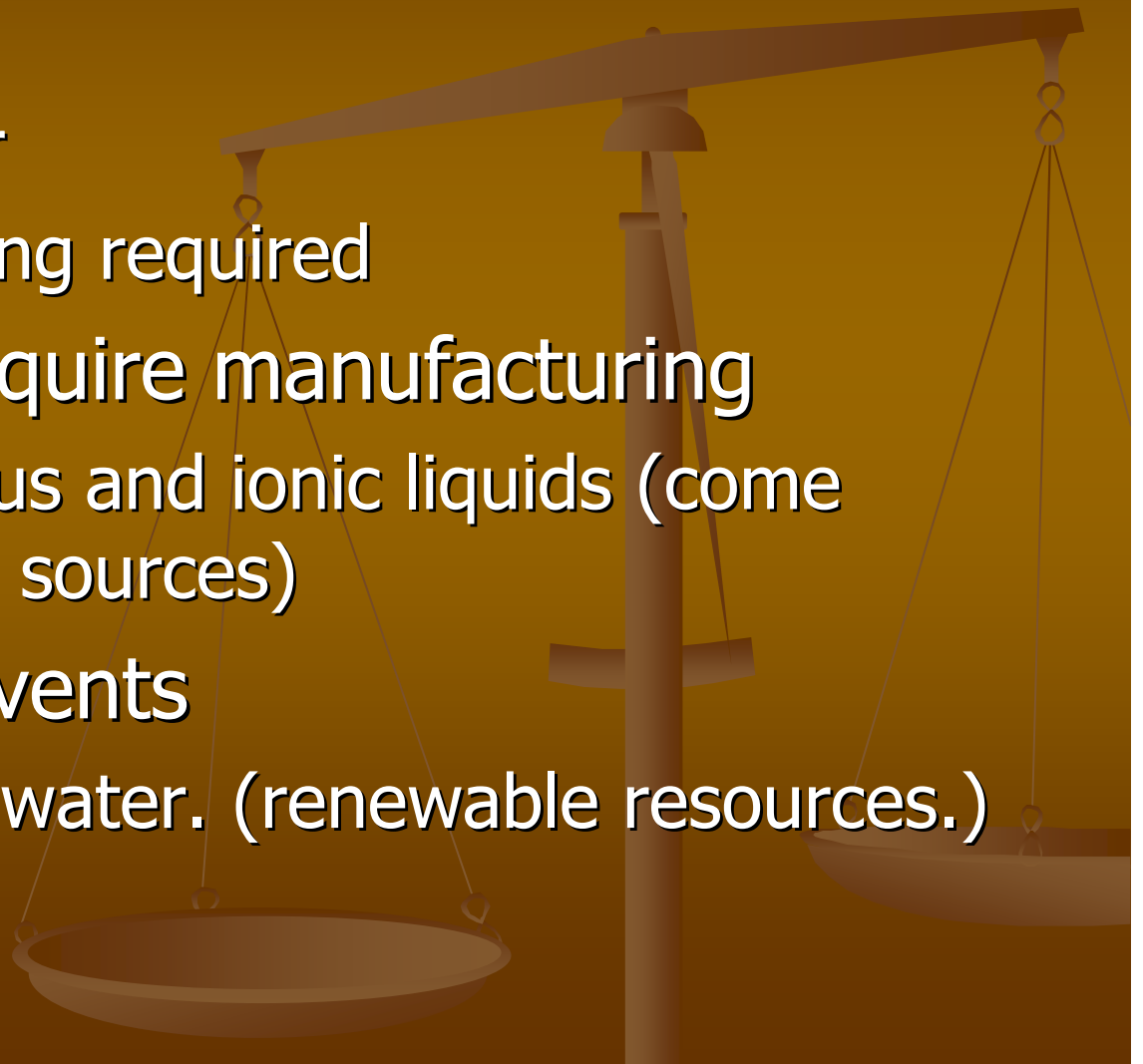
CO₂ as an Alternative Solvent

- Classification of Green Solvents (Clark and Tavener)
 - Manufacturing
 - Distribution
 - Use
 - Disposal



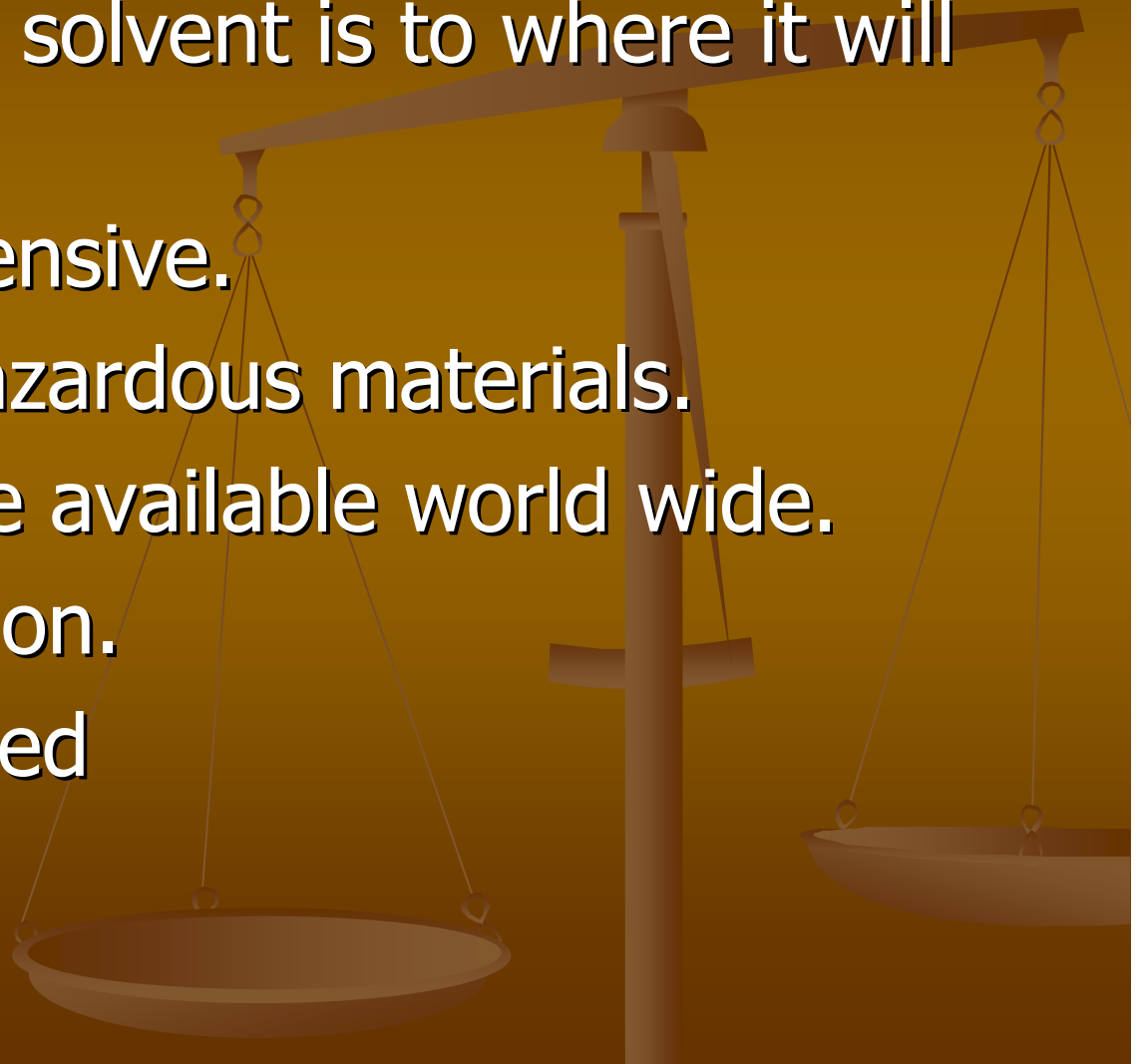
Manufacturing

- Ranks well
 - Similar to water
 - No manufacturing required
- Solvents that require manufacturing
 - Acetone, fluoruous and ionic liquids (come from petroleum sources)
- Other green solvents
 - Bioethanol and water. (renewable resources.)



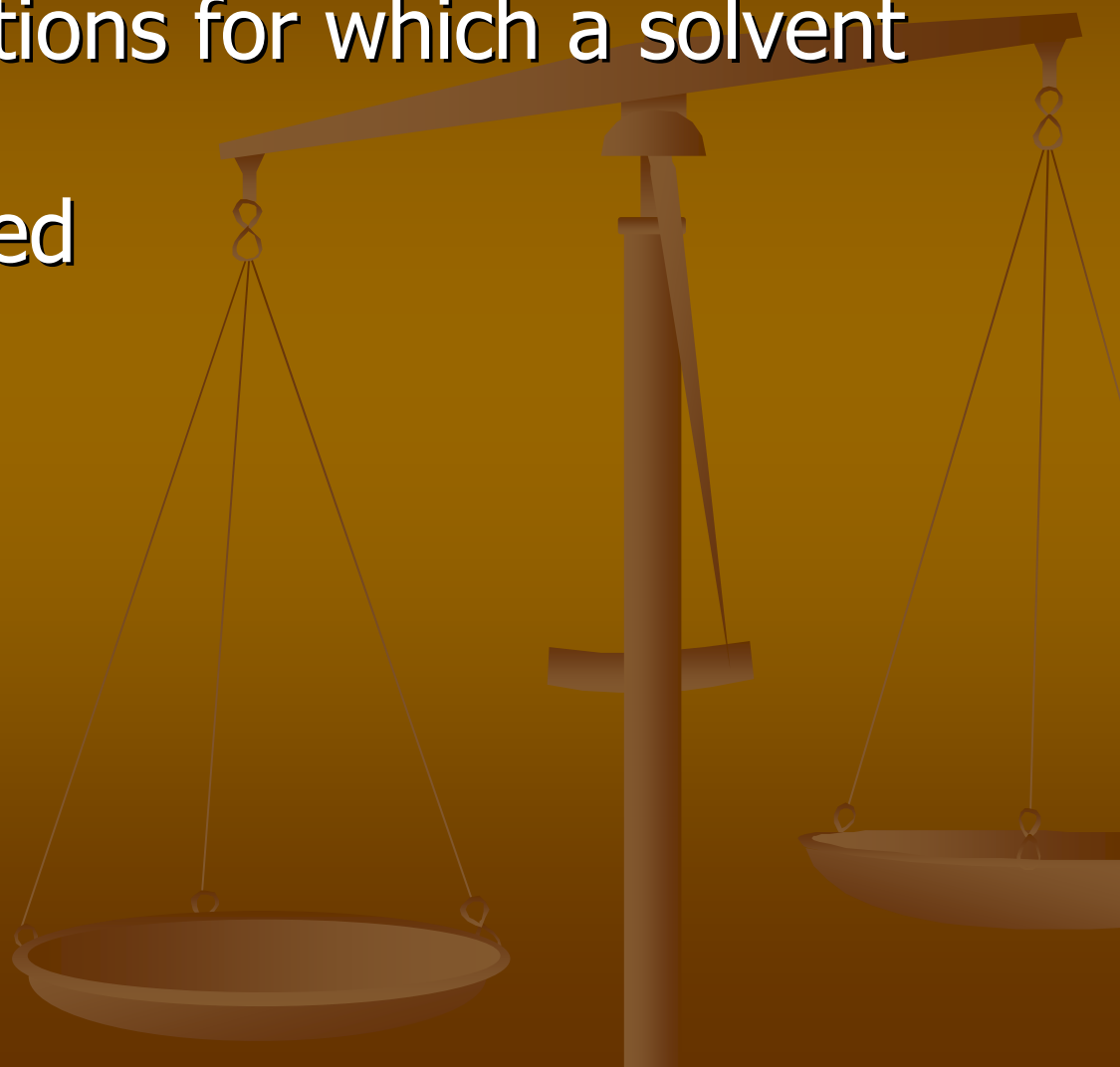
Distribution

- How available a solvent is to where it will be used.
- Shipping is expensive.
- Transporting Hazardous materials.
- CO₂ and H₂O are available world wide.
- On site production.
- Used and recycled



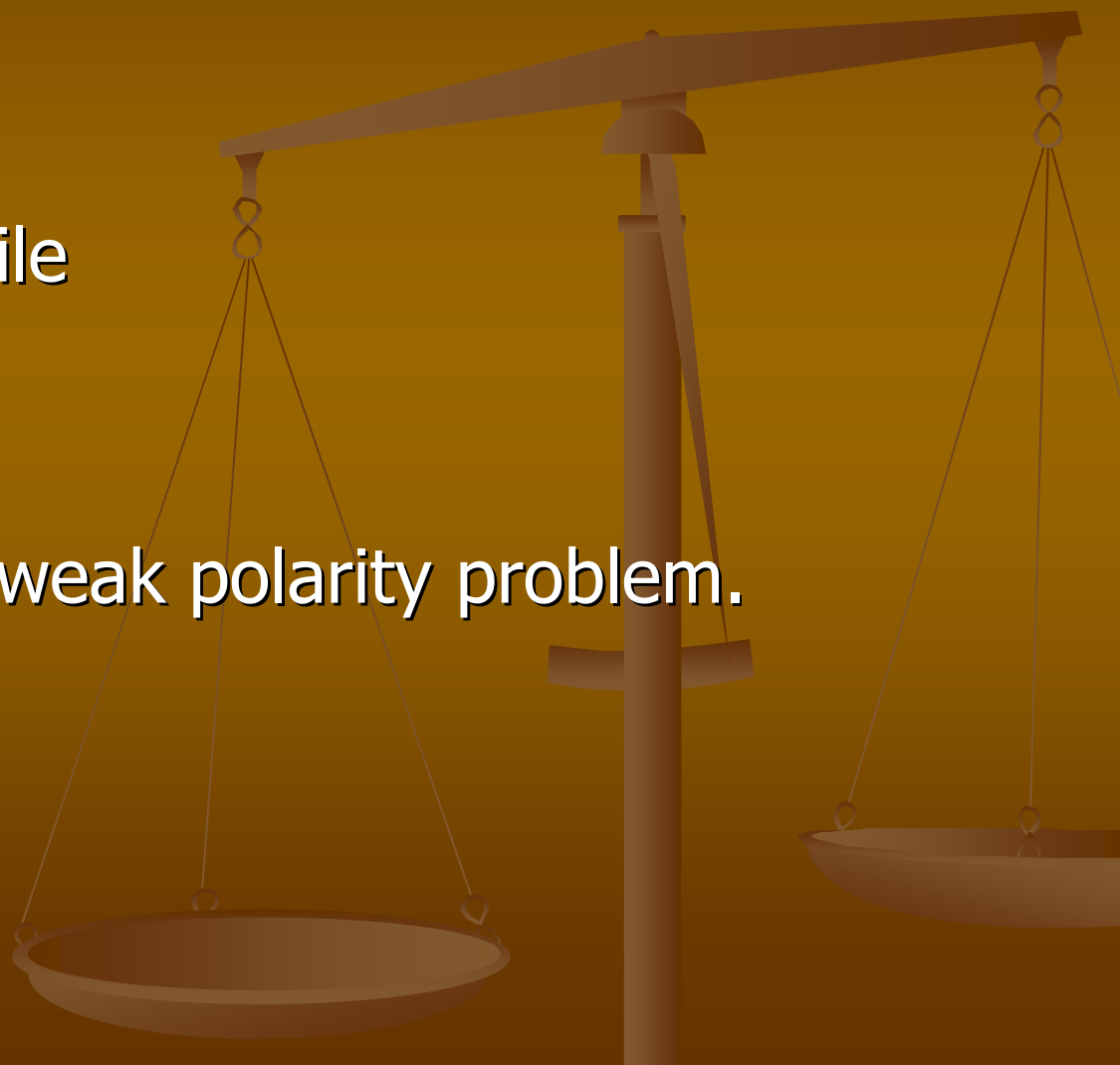
Solvent Use

- Number of reactions for which a solvent can be used.
- More Complicated
 - Polarity
 - Viscosity
 - Density
 - M.P. B.P.
 - Volatility
- Algorithms



CO₂ Use as Solvent

- CO₂
 - Weak polarity
 - Extremely volatile
 - Relatively Inert
 - Not flammable
 - Attempts to fix weak polarity problem.



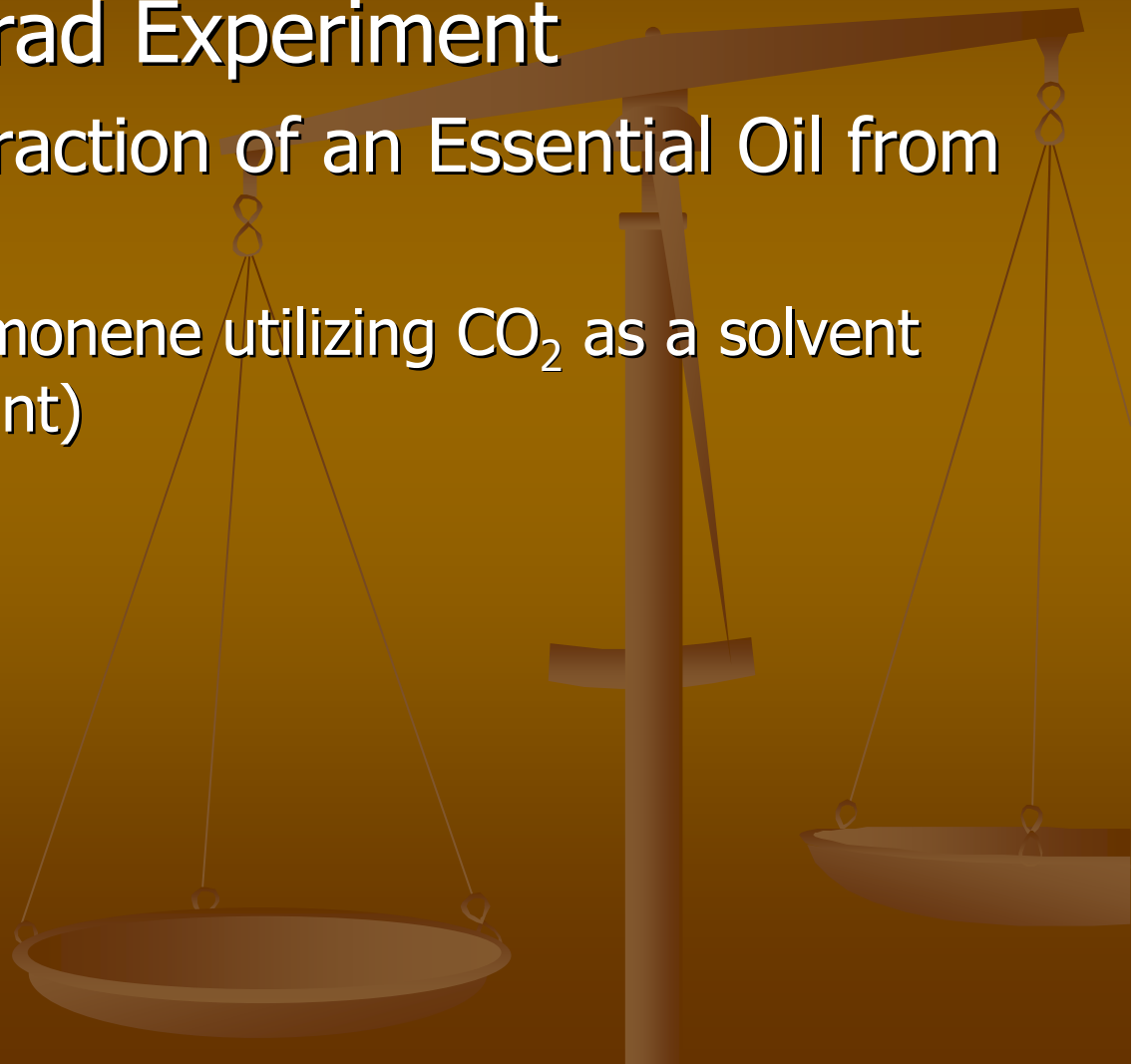
Disposal

- Released into the environment
 - Vented directly
 - Large Scale (fermentation) recovered and reused
 - Collected and reused
- Other solvents
 - Incinerated
 - Other high energy means of disposal



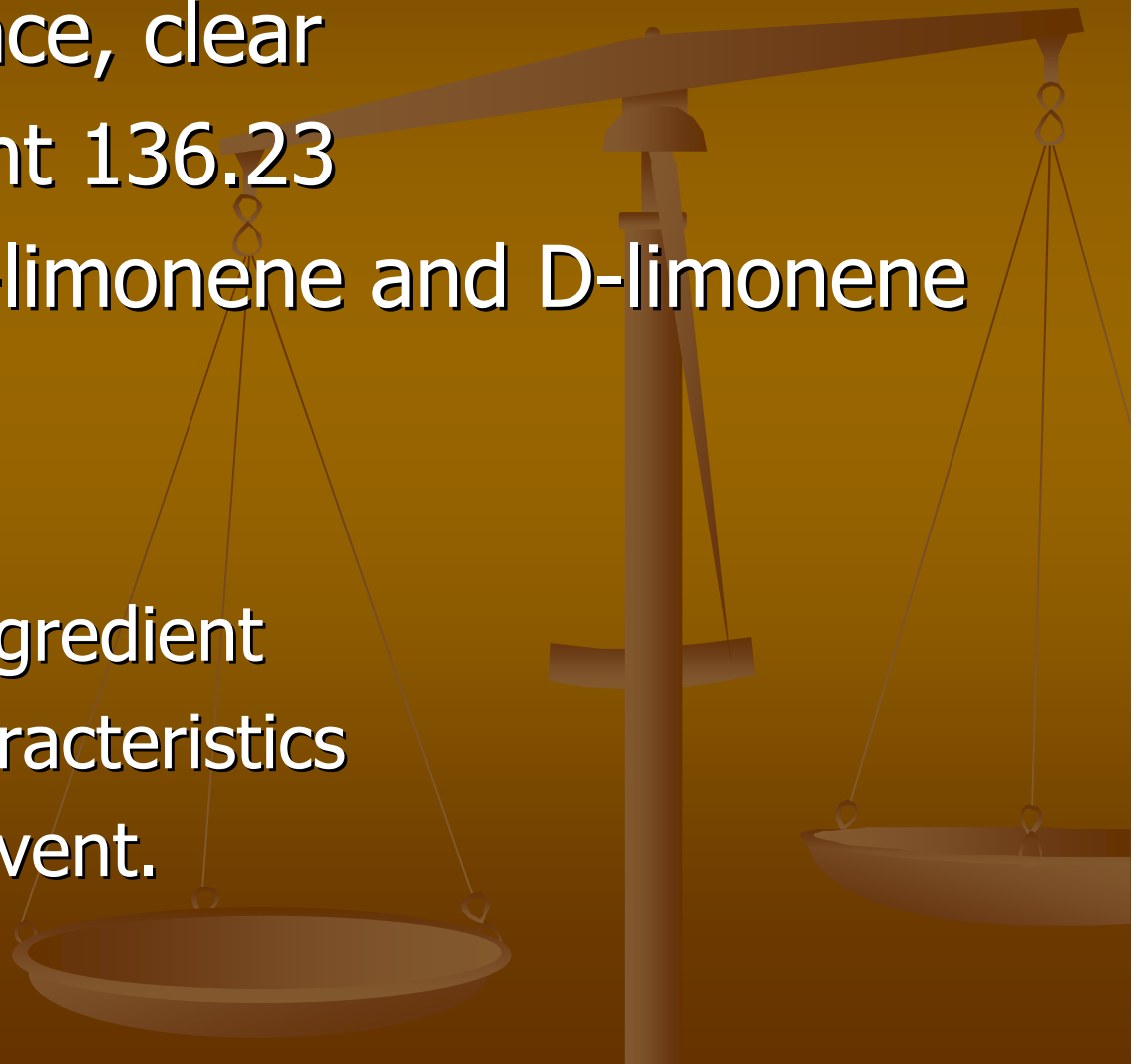
Limonene Extraction Expansion

- Original undergrad Experiment
 - “Liquid CO₂ Extraction of an Essential Oil from Orange Rind.”
 - Extraction of limonene utilizing CO₂ as a solvent (at its triple point)

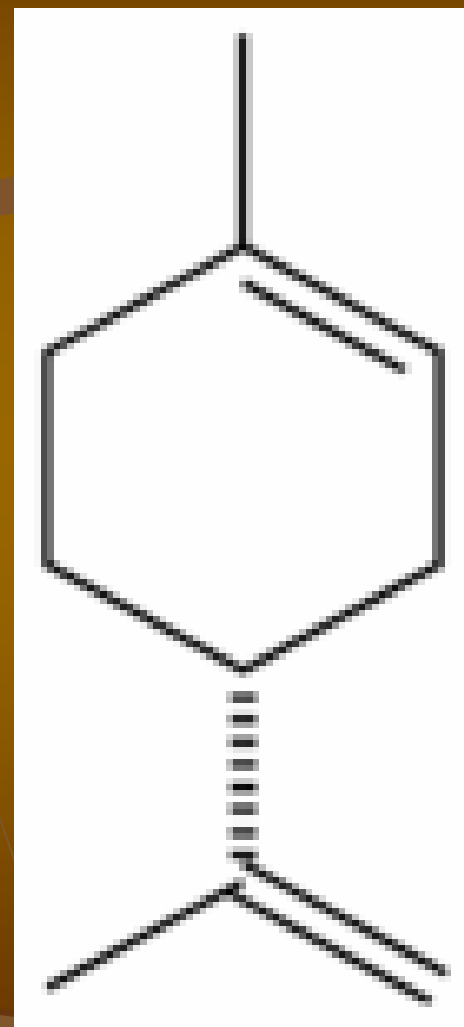
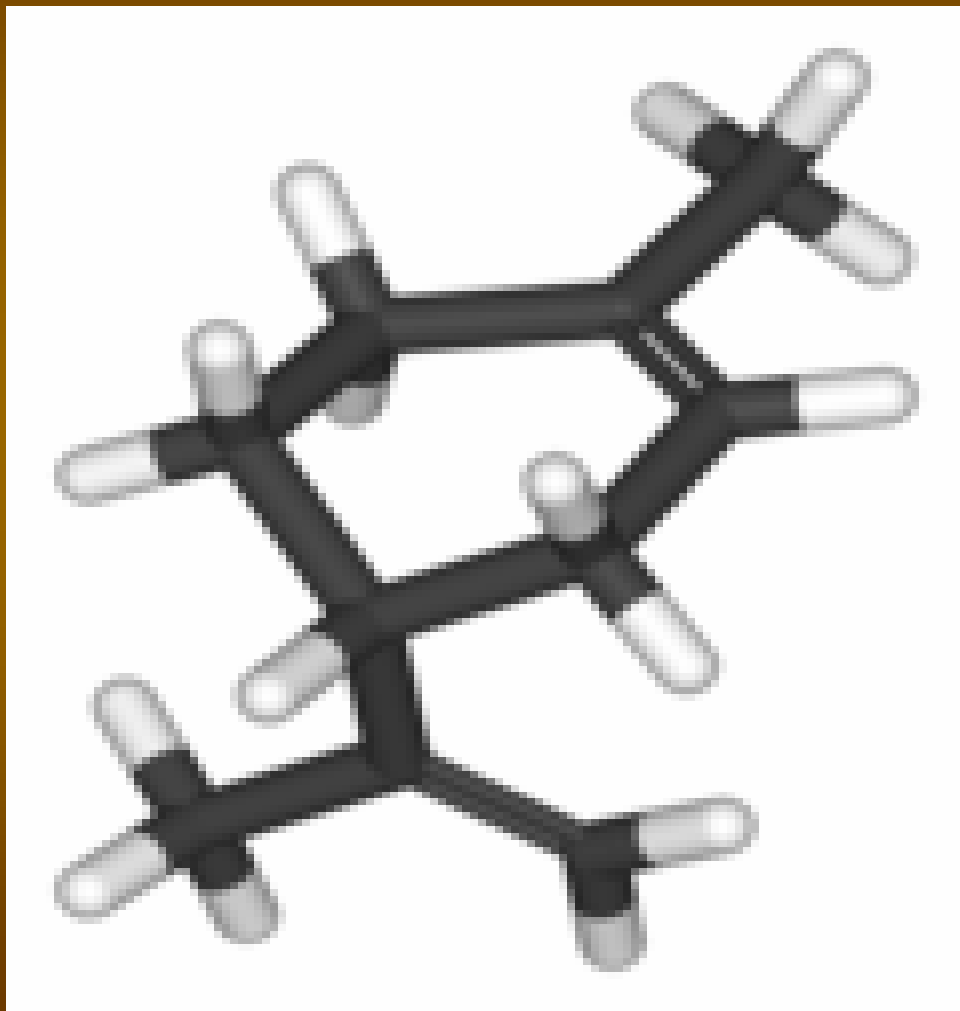


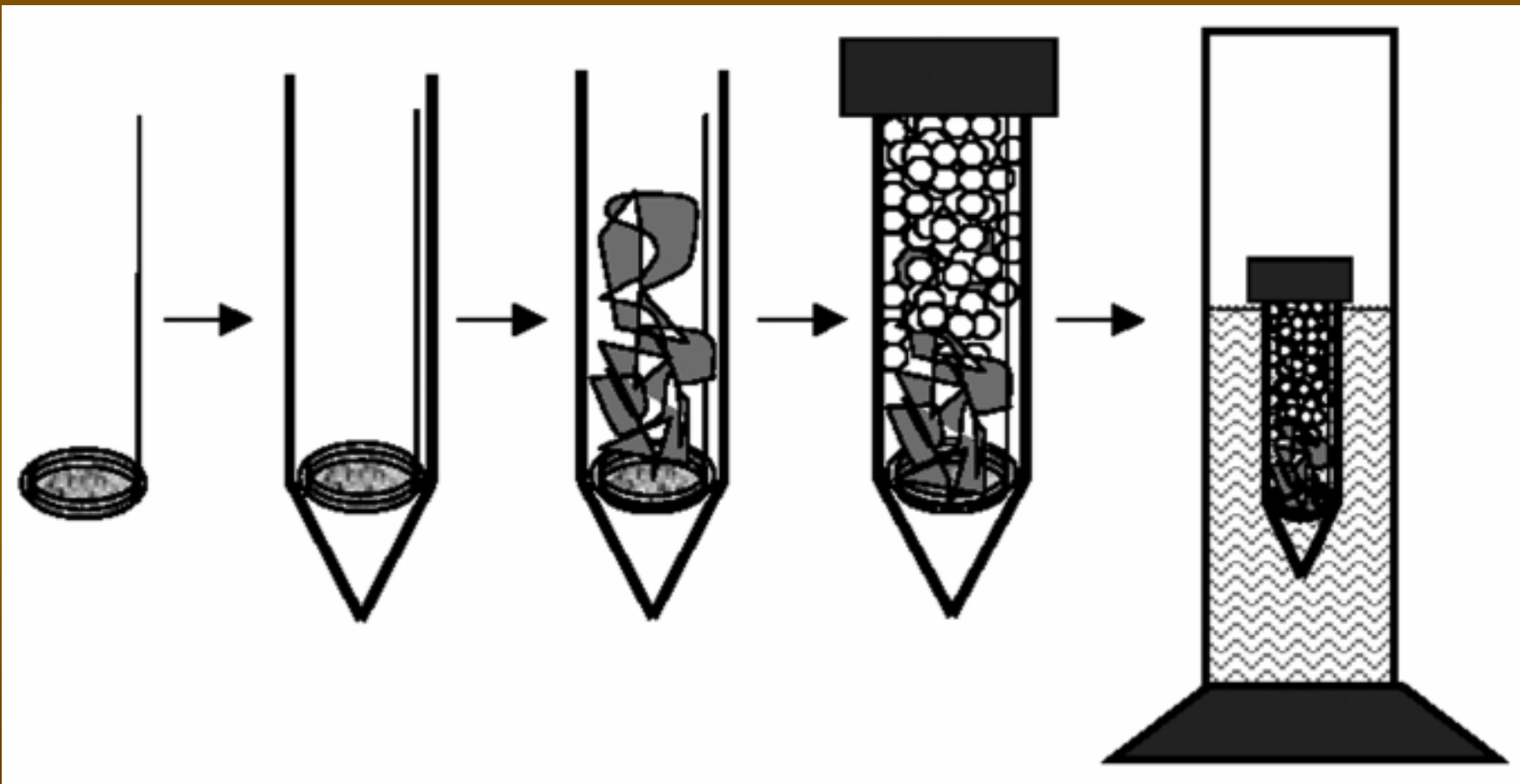
Limonene

- As pure substance, clear
- Molecular Weight 136.23
- Optical forms L-limonene and D-limonene
- Aromas
- Uses
 - Air freshener ingredient
 - Anti-cancer characteristics
 - Cleaner and solvent.

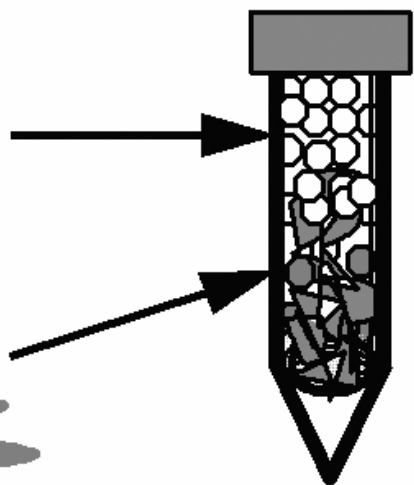
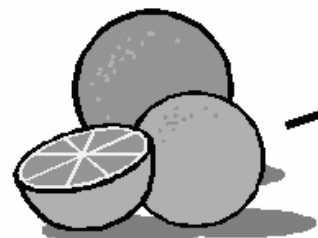


Limonene



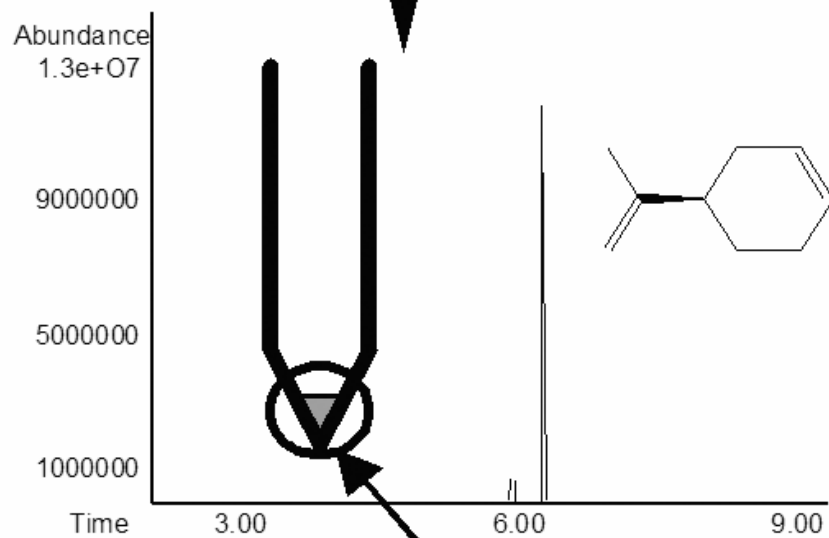


Dry Ice

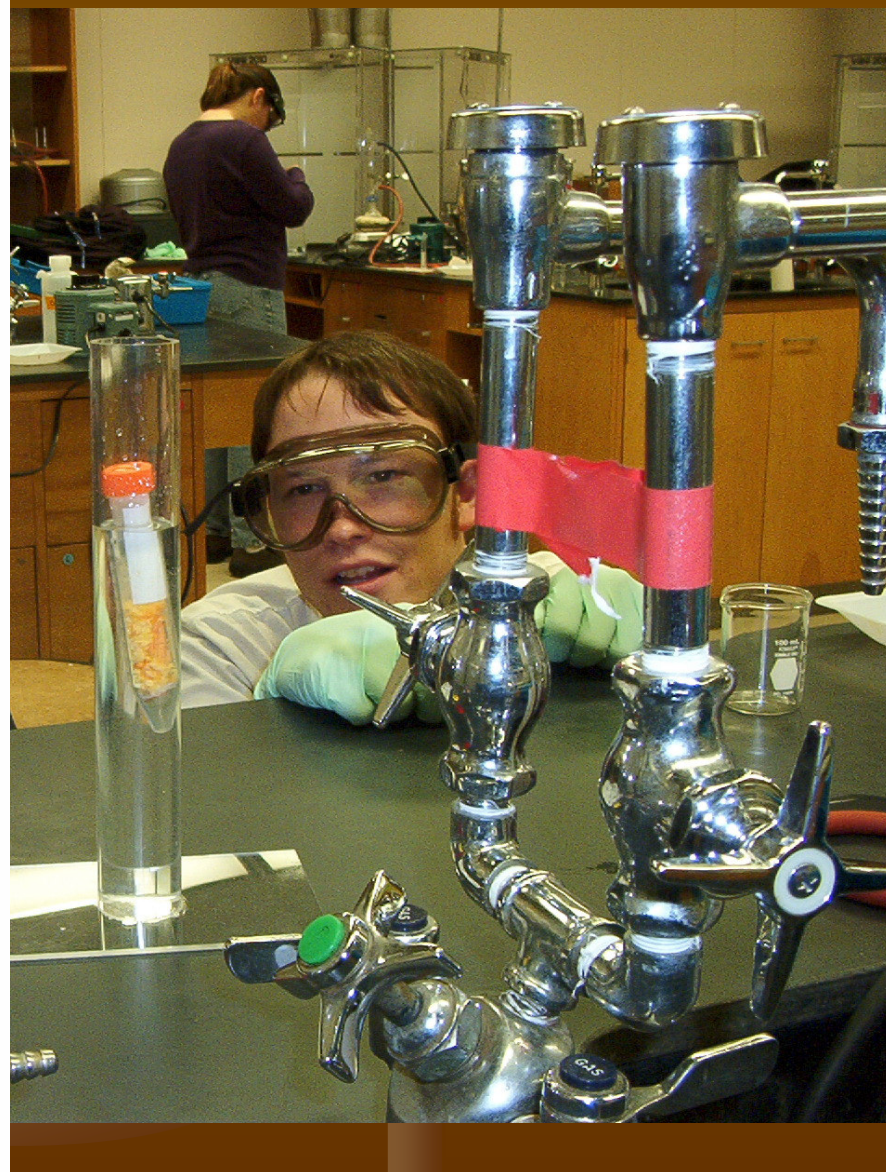


1) Liquid CO₂
Extraction

2) CO₂ evaporation
3) Rind removal

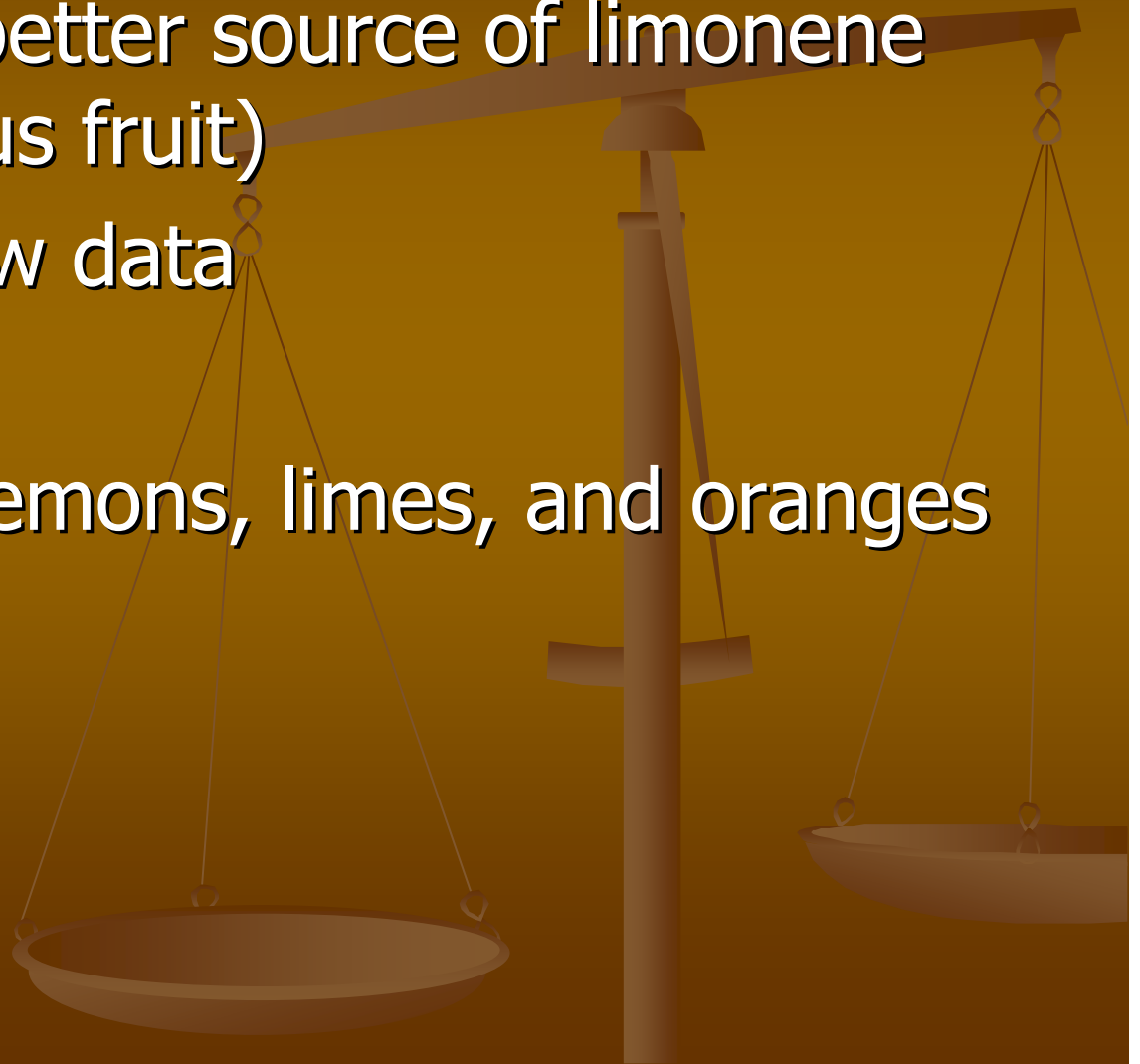


D-limonene



Expansion

- Object: Find a better source of limonene (a different citrus fruit)
- Produced all new data
- Procedure
- Utilized use of lemons, limes, and oranges



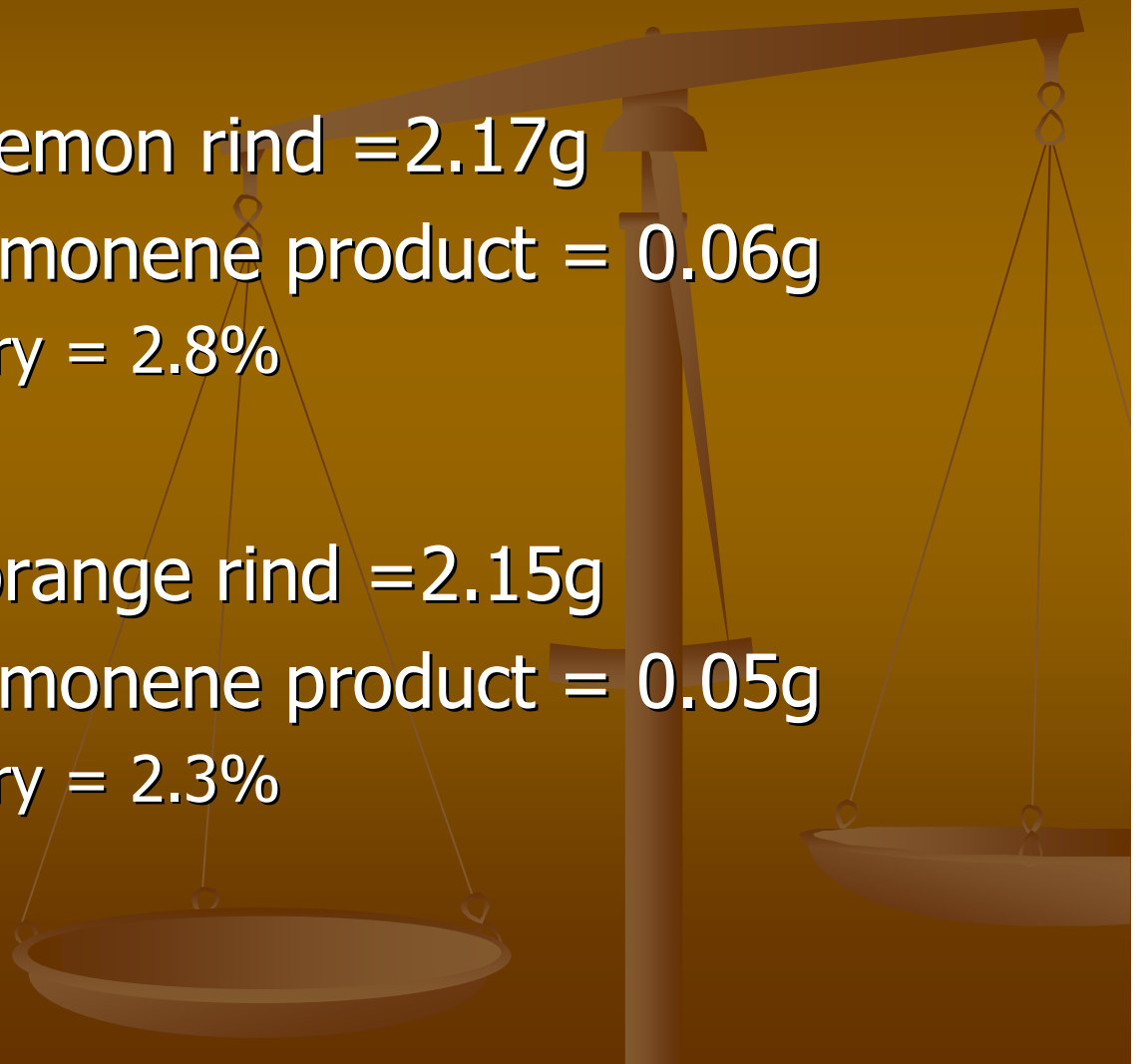
Results

■ Lemon

- Avg Weight of lemon rind = 2.17g
- Avg weight of limonene product = 0.06g
 - Percent recovery = 2.8%

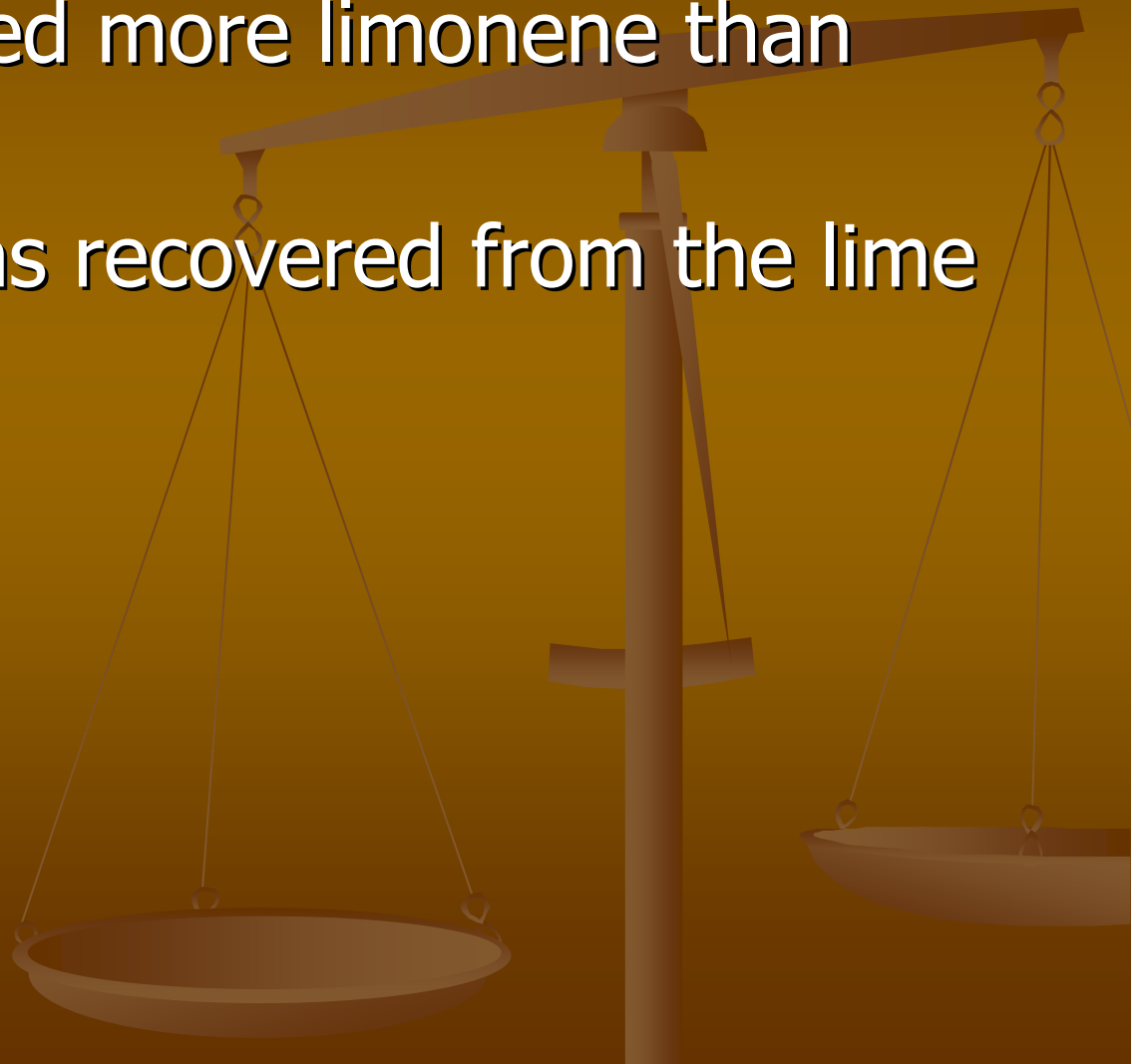
■ Orange

- Avg weight of orange rind = 2.15g
- Avg weight of limonene product = 0.05g
 - Percent recovery = 2.3%



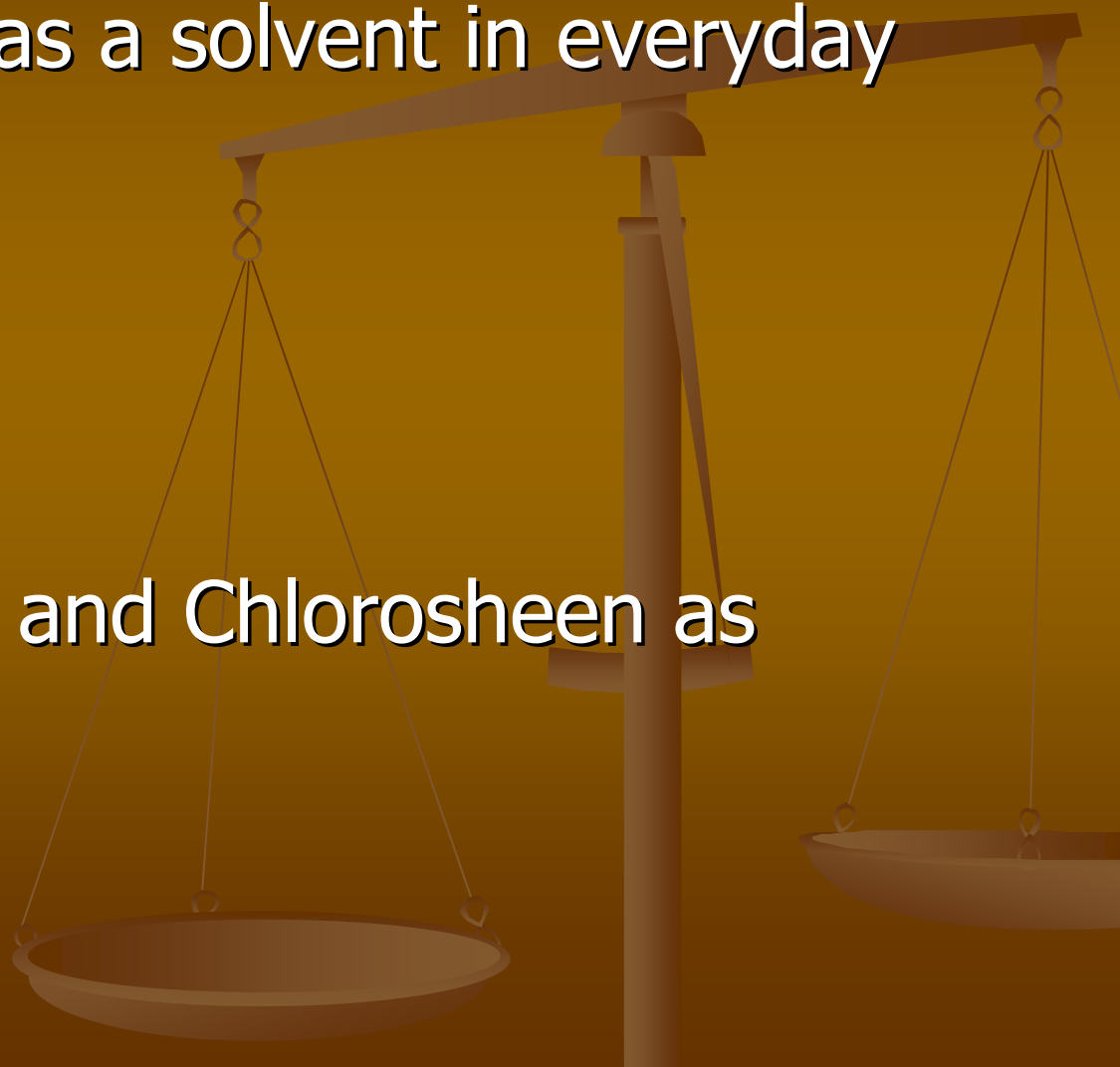
Results Cont'd

- Lemons produced more limonene than oranges.
- No limonene was recovered from the lime samples.



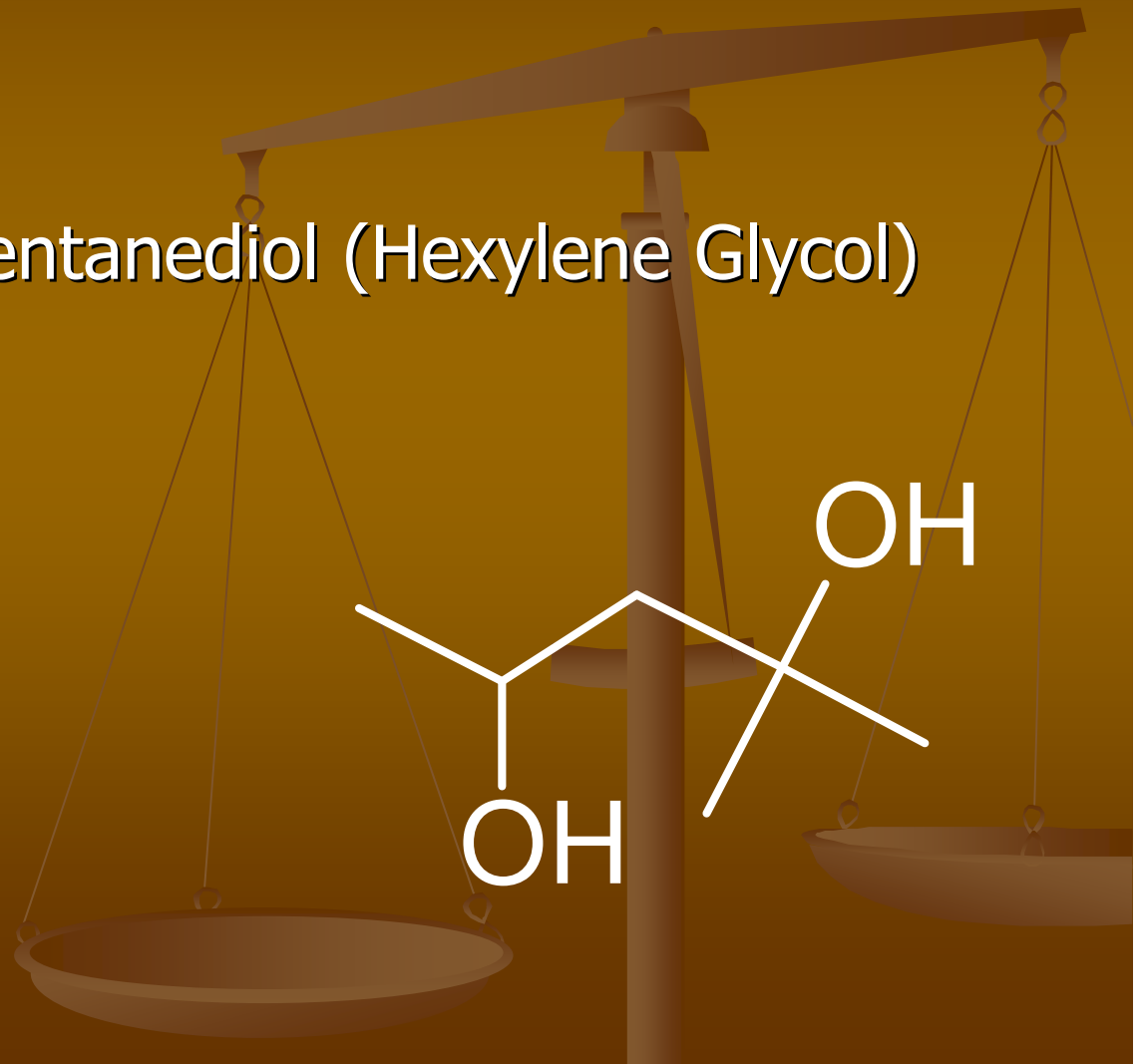
Test Tube Dry Cleaning

- Exploring lqCO_2 as a solvent in everyday use.
 - Dry cleaning
- Four Clothes
- Four Stains
- lqCO_2 as solvent and Chlorosheen as detergent



Chlorosheen

- Composed of:
 - Pale Oil
 - 2-methyl-2,4-pentanediol (Hexylene Glycol)



Materials

- Clothes
 - Cotton
 - Nylon
 - Polyester
 - 60%nylon/40%rayon
- Stains
 - Ketchup
 - Mustard
 - Ink
 - Highlighter



Results

Ketchup

Mustard

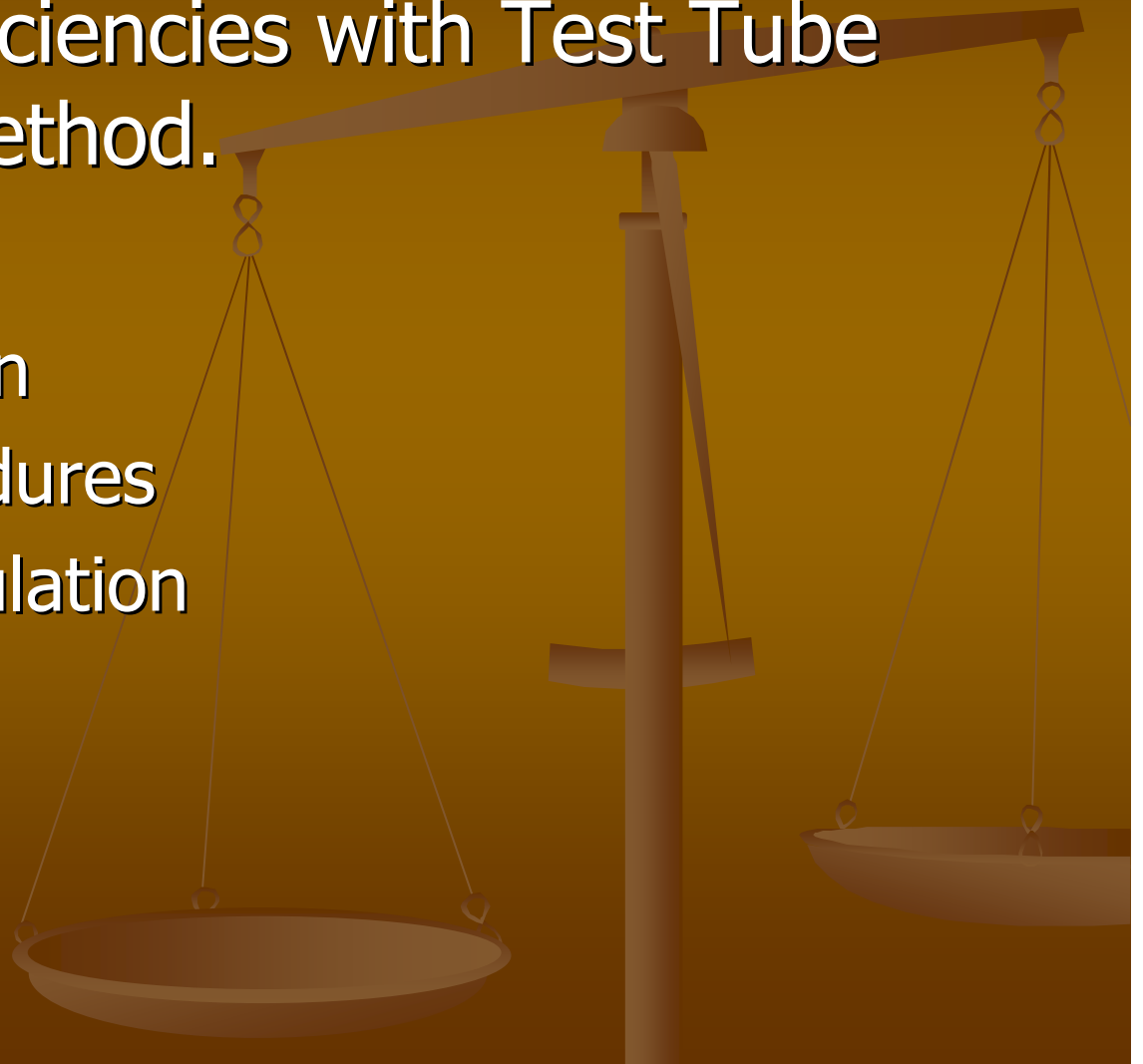
Ink

Highlighter

	Before	After	Before	After	Before	After	Before	After
Cotton	5	1.5	6	3	5	1	5	2
Nylon	4	1	6	3	5	1	4	1
Polyester	3	2	6	5	5	3	5	0
60/40	3	0	3	1	4	4	3	0

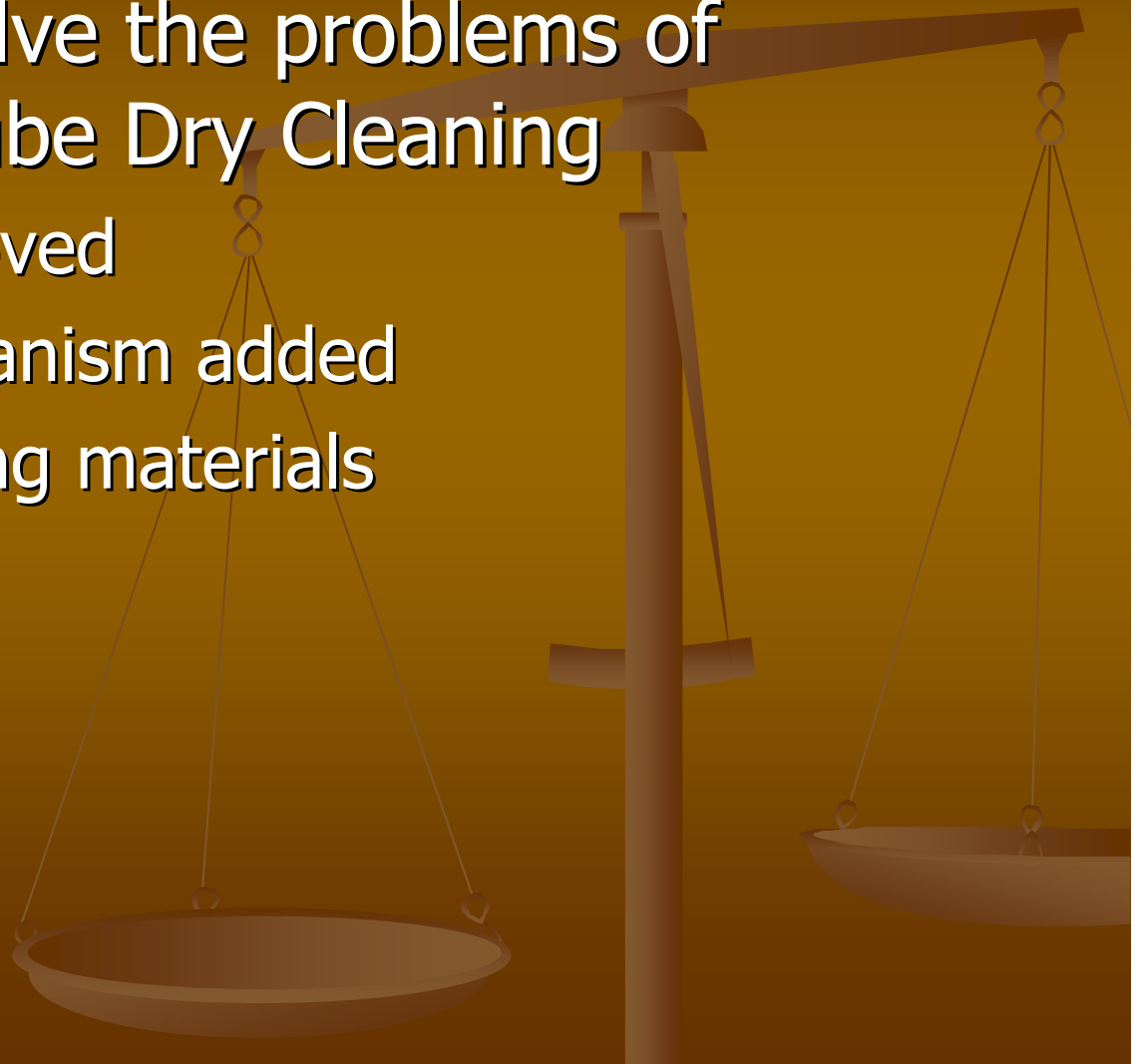
Drawbacks

- There were deficiencies with Test Tube Dry Cleaning method.
 - Lack of agitation
 - Washing procedures
 - Physical Manipulation



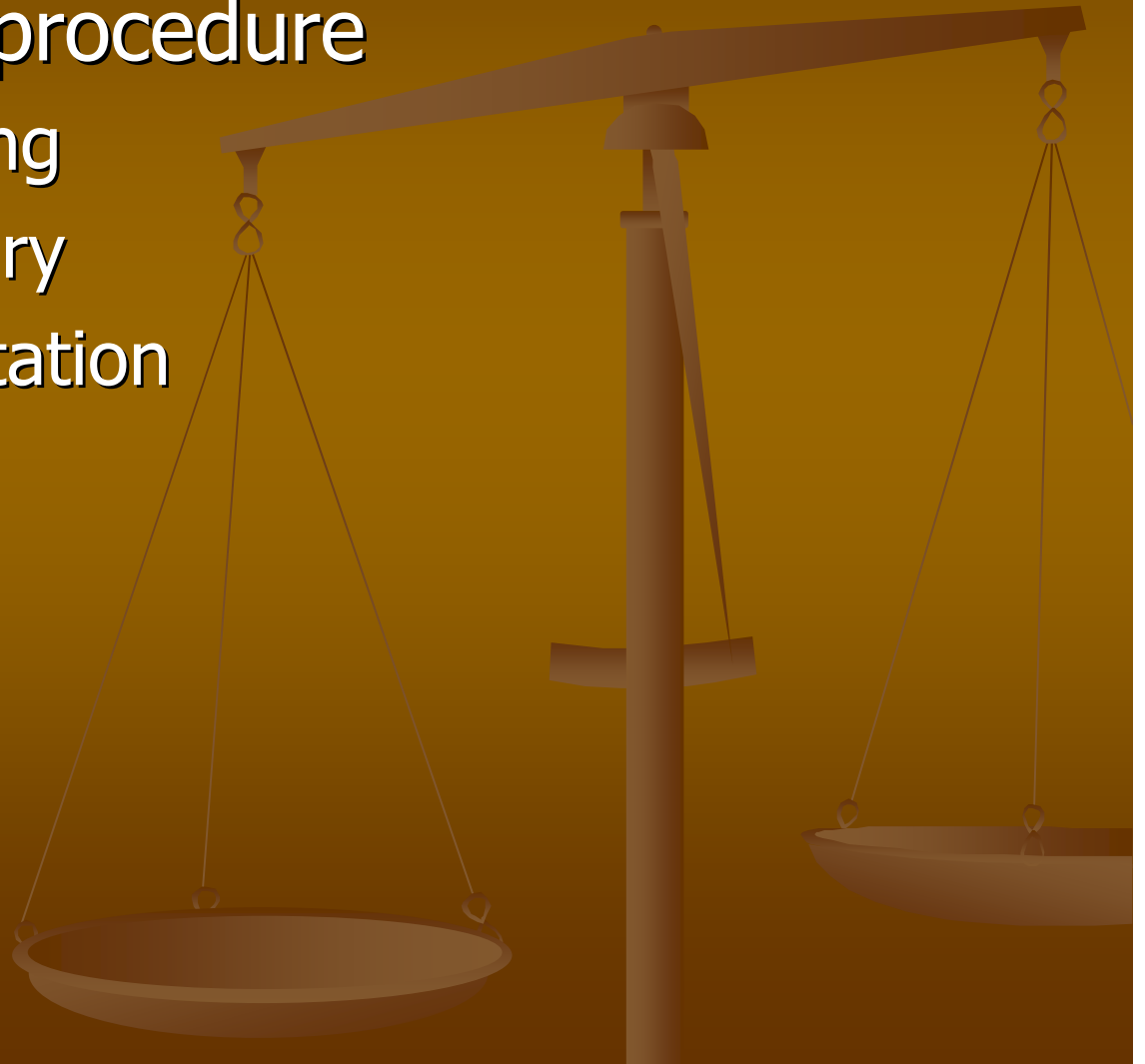
Test Tube Dry Cleaning (Improved)

- Produced to solve the problems of Original Test Tube Dry Cleaning
 - Metal Coil removed
 - Agitating mechanism added
 - Different staining materials



Test Tube Dry Cleaning (Improved)

- Followed same procedure
 - No more washing
 - Allowed to air dry
 - No physical agitation



Results

Ketchup

Dry Erase

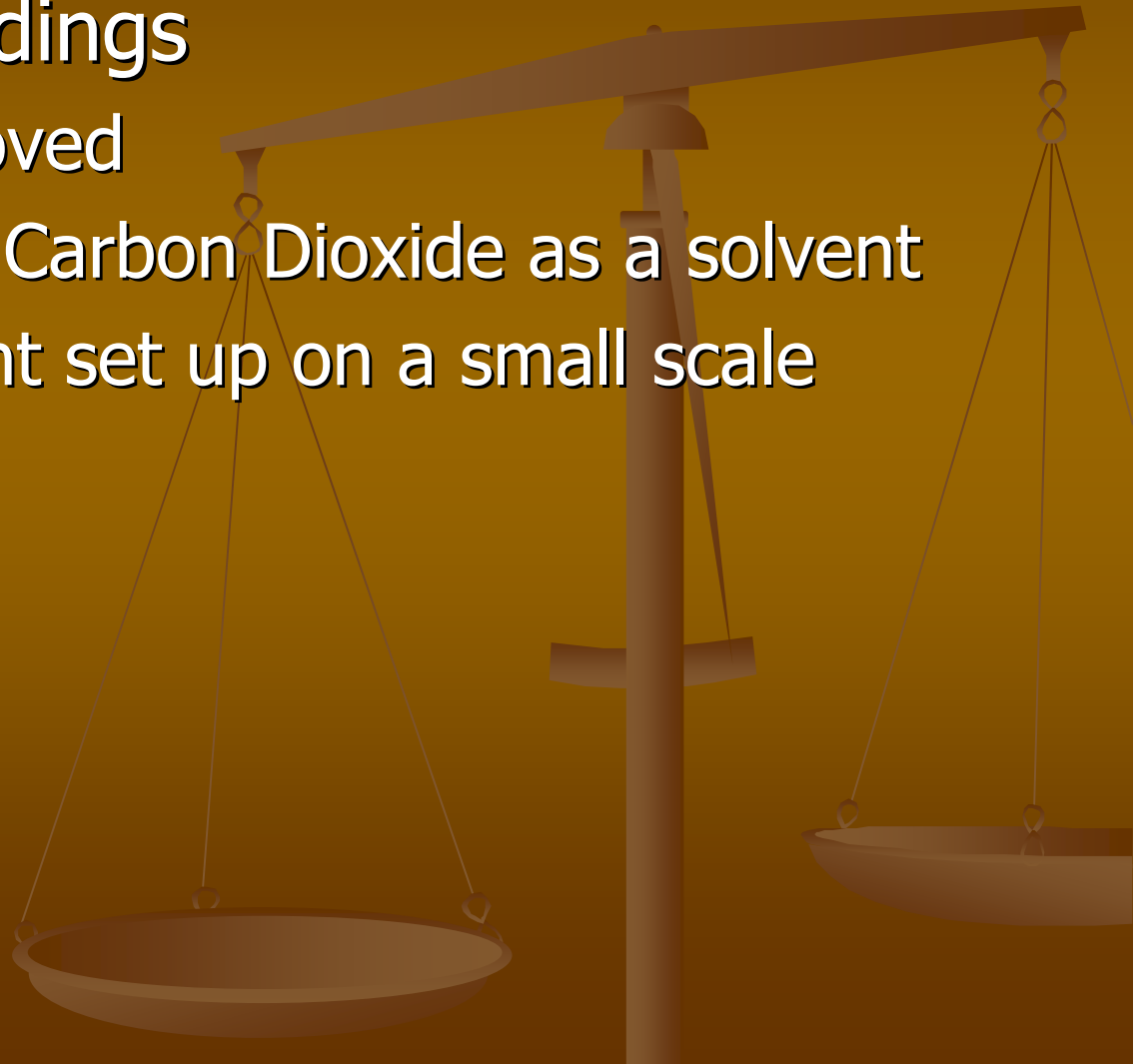
Highlighter

Pen

	Before	After	Before	After	Before	After	Before	After
Cotton	5	2	6	4	5	3	8	6
Nylon	4	1	6	5	4	3	7	7
Polyester	5	1	6	5	4	3	8	7
60/40	1	0	3	3	2	0	5	3

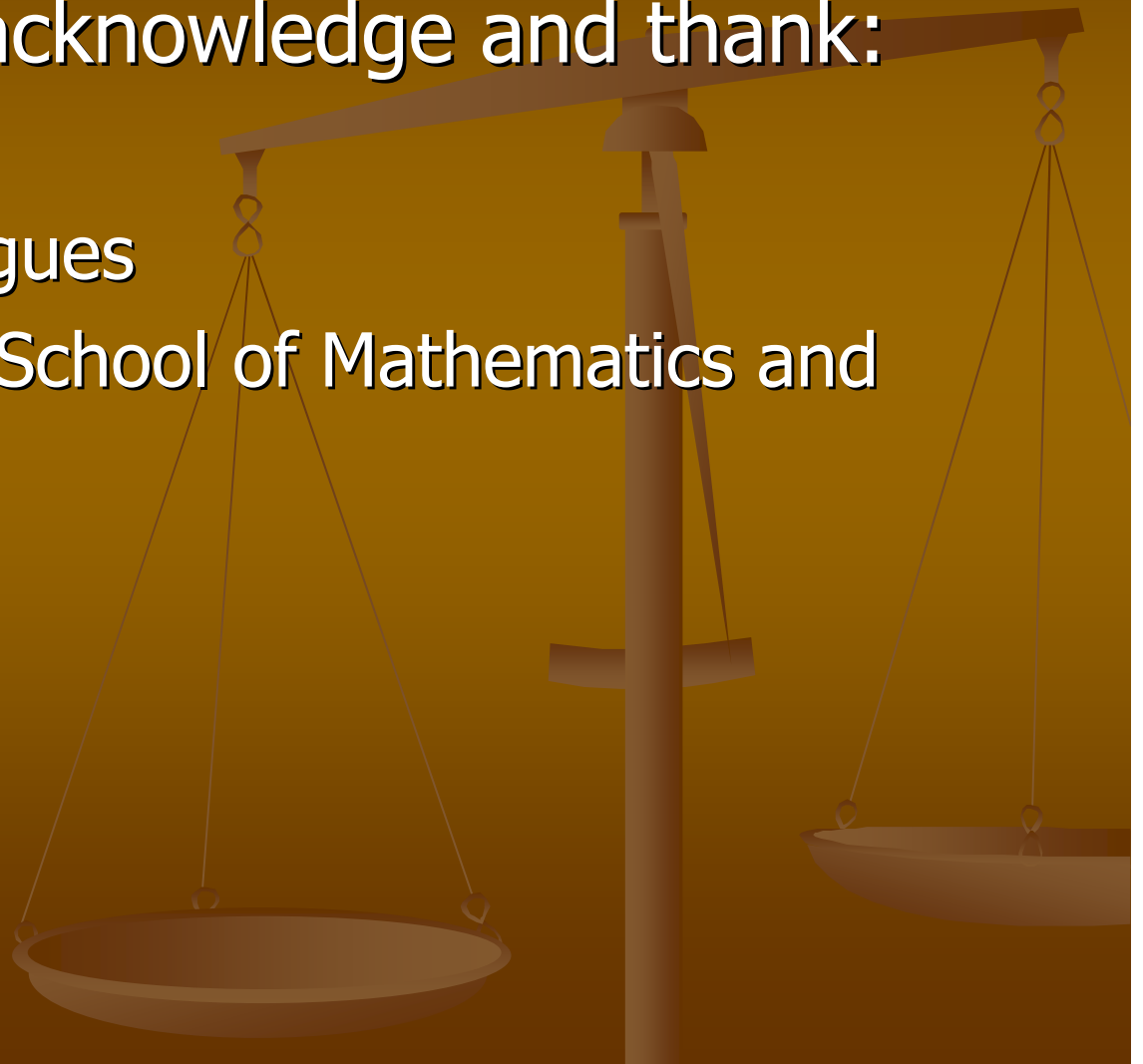
Conclusion

- Inconclusive findings
 - Stains not removed
 - Not capacity of Carbon Dioxide as a solvent
 - Lack of sufficient set up on a small scale



Special Thanks

- I would like to acknowledge and thank:
 - Dr. Carl Lecher
 - CHE 498 colleagues
 - Marian College School of Mathematics and Sciences



Questions?



Sources

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- Clark, James H., Tavener, Stewart T., Alternative Solvents: Shades of Green. Organic Process Research & Development, Green Chemistry Centre, Department of Chemistry, University of York Heslington, York U.K. 149, 2007.