Soaps, Detergents, and Personal Care Products

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Non-major courses taught

- **CHM 121IN, Chemistry and Society**
  - **Took over course in 2003.**
  - **No textbook, only my notes and Internet resources as of 2004**
- **CHM 125IN, Consumer Chemistry**
  - **Originated course in 2003**
  - **Textbook: Selinger, Ben, *Chemistry in the marketplace*.**
  - **No textbook, only my notes and Internet resources as of 2009**
- **These are taught as integrated hands-on courses.**
- **Classes meet in the lab (2 hours, 40 minutes)**
  - **30 to 45 minutes lecture followed by hands-on activities and experiments with some intermittent discussions**

Topics for CHM 125IN: Consumer Chemistry

- Basic chemistry
  - Elements, compounds, measurement, chemical formulas, acids and bases, chemical reactions, intro to organic compounds (includes petroleum products).
- Lab safety and introduction to toxicology
- Chemistry in the laundry
  - Soaps, detergents, cleaning aids
- Chemistry in the kitchen
  - Cooking, foods, food additives, flour and bread, molecular gastronomy
- Water
- Chemistry in the boudoir
  - Perfumes, skin creams, sunscreens, OTC medications
- Materials
  - Polymers, glass, metals, fabrics, paper, artist materials
- Introductory nanotechnology

Main Objective

Students must be able to locate information, read and understand it, and have the knowledge to make intelligent, rational decisions regarding the accuracy of that information to become informed, active citizens in today's world.

- **These students are our future.**
- **They go beyond scientists and engineers.**
- **They will be our:**
  - **Legislators**
  - **CEO's**
  - **Business people**
  - **Military officers, with power over and responsibility for another generation of young soldiers handling the world's most sophisticated weapons systems**
  - **First responders – fire fighters/police officers/hazardous materials specialists**
  - **Sports coaches and scout leaders**
  - **Parents of our brilliant & beautiful grandchildren**
  - **Our future sources of funding and support**

Selected Class Topics

Water testing (as part of introductory environmental chemistry)

Mainly drinking water:

- Tap water
- Bottled water
- Filtered water (Britta)

Use Hach test kits:

- pH
- Hardness
- Iron
- Chlorine: Free and total
- Copper: Free and total
- Lead
- Dissolved solids
- Arsenic (well water only)

Soap and Detergent

Preparation of a soap

Start with lard or vegetable oil.
(I think lard makes the best soap.)

Preparation of detergent

Prepare sodium dodecylsulfate.
Preparation while saponification is running.

Properties of soaps and detergents

Emulsifying properties
Behavior in hard water
Alkalinity
Reaction with mineral acid

Testing detergents

Testfabrics, Inc. sells “standard” stained cloth to test effectiveness of detergents.

These tend to be expensive. Even “seconds” are too expensive for classroom use.

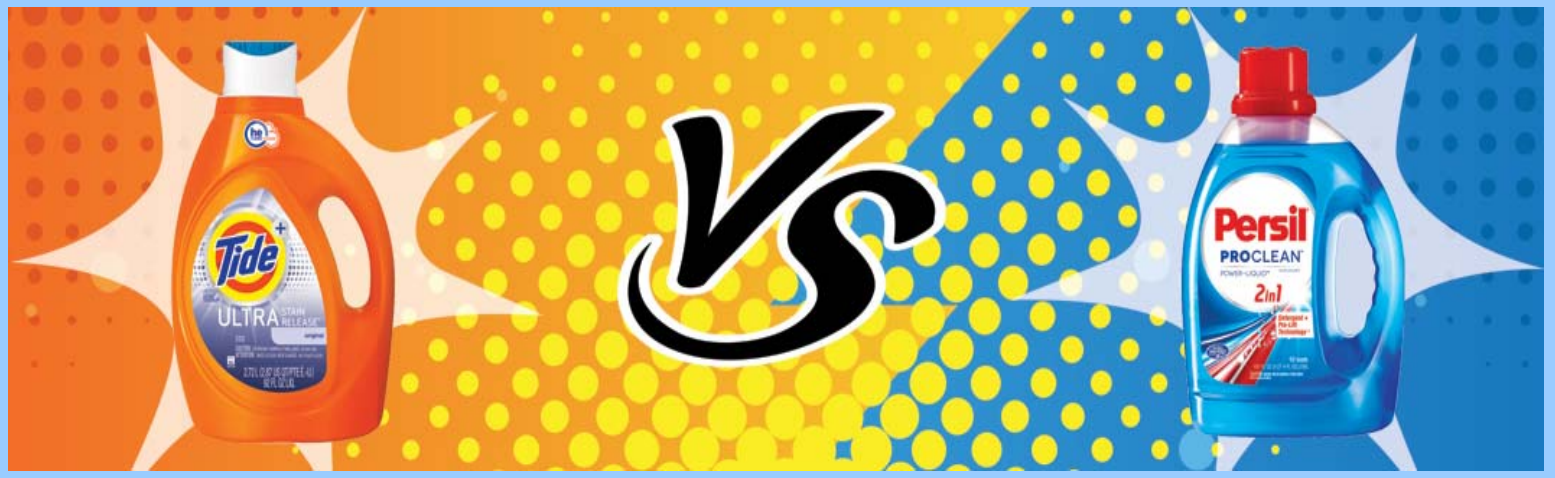
Home made stained fabric

Use cotton cloth, 12 x 12 inches (30 x 30 cm)

Stain with:

- Make-up
- Lipstick
- Red wine or grape juice
- Ketchup or tomato sauce
- Mustard
- Egg
- Butter
- Baby food or jelly/jam
- Chocolate or cocoa
- Tea or coffee
- Soy sauce
- Grass or plant leaves
- Clay or soil (mud)
- Grease or used engine oil
- Ink (ball point pen)

Wash with detergent (with and without additives)



Ingredients unique to Tide | *Purpose* **| Manufacturers**

Monoethanolamine citrate | *Soil-capturing, -buffering agent* | Created in situ

Diethylene glycol | *Solvent* | Dow Chemical, LyondellBasell, Shell

Polyethyleneimine propoxyethoxylate | *Soil-release or -capturing polymer* | BASF

Sodium cumene sulfonate | *Emulsifying and dispersing agent* | Nease, Stepan

Diethylenetriaminepentaacetic acid | *Chelating agent* | BASF, Dow Chemical

Disodium diaminostilbene disulfonate | *Optical brightener that makes clothes appear brighter by absorbing UV light and reemitting it in the blue region* | Archroma, BASF

Calcium formate | *Enzyme stabilizer* | GEO Specialty Chemicals, Perstorp

Glucanase | *Enzyme that breaks down polysaccharide-based soils and stains* | DuPont, Novozymes

Ingredients unique to Persil | *Purpose* **| Manufacturers**

Alcohol ethoxylate | *Low-foaming surfactant* | Huntsman, Sasol, Shell

Sodium citrate | *Builder and chelating agent* | Archer Daniels Midland, Cargill

Trisodium ethylenediamine disuccinate | *Chelating agent* | Innospec

Tetrasodium ethylenediamine tetraacetic acid | *Soil-capturing agent* | AkzoNobel, BASF, Dow Chemical

Lipase | *Enzyme that breaks down fat-based soils and stains* | DuPont, Novozymes

Cellulase | *Enzyme that removes soils from cotton and improves cotton's softeness and color brightness* | DuPont, Novozymes

Disodium distyryl biphenyl disulfonate | *Optical brightener that makes clothes appear brighter by absorbing UV light and reemitting it in the blue region* | BASF

Ingredients in common | *Purpose* | **Select Manufacturers**

Water | *Process aid*

Alcohol ethoxysulfate | *Premium surfactant especially effective in hard water* | Pilot Chemical, Stepan

Alkylbenzene sulfonate | *Low-cost general-purpose surfactant* | Huntsman, Pilot Chemical, Stepan

Sodium fatty acids (soap) | *Traditional surfactant* | P&G Chemicals, Twin Rivers Technologies

Polyethylenimine ethoxylate | *Soil-release or -capturing polymer* | BASF

Propylene glycol | *Solvent and enzyme stabilizer* | Dow Chemical, Huntsman, LyondellBasell

Protease | *Enzyme that breaks down protein-based soils and stains* | DuPont, Novozymes

Sodium borate | *Soil-capturing agent, enzyme stabilizer* | Rio Tino Borates, Searles Valley Minerals

Ethanol | *Process aid that keeps ingredients in solution* | Archer Daniels Midland, Cargill, Grain Processing

Fragrance | *Scent* | Multiple

Amylase | *Enzyme that breaks down starch-based soils and stains* | DuPont, Novozymes

Sodium formate | *Balances electrolytes* | BASF, Perstorp

Mannanase | *Enzyme that breaks down guar gums, used as thickeners in ice cream, salad dressing, and other foods* | DuPont, Novozymes

Polydimethylsiloxane (dimethicone) | *Defoaming agent* | Dow Corning

Blue dye | *Colorant* | Multiple

Note: Ingredients are listed roughly in order of relative volume.

Reference: Chemical & Engineering News, January 23, 2017

http://cen.acs.org/articles/95/i4/PG-Henkel-head-head-laundry.html

Dye Catcher

Absorbs loose dyes which bleed from clothes in the wash and prevents them from running onto other clothes.

Composed of a piece of white fabric treated with soda ash, Na_2CO_3 , (washing soda) solution.

Make your own dye catcher

Add 30 g Na_2CO_3 (Washing soda) to 500 mL water. Stir to dissolve.

Add 15 cm square pieces of felt or an old wash cloth to the solution.

Soak for several minutes.

Remove fabric pieces and wring out excess liquid.

Allow fabric pieces to dry.

Washing soda, sodium carbonate, is used to fix dyes to cloth in the dyeing process

Washing soda is a water softener. It is used as a “builder”, along with zeolites and complexing agents, in laundry detergents.

Fabric softeners (fabric conditioners)

- Usually added to the wash during the rinse cycle.
- Fabric softeners coat the surface of a fabric with chemical compounds that are electrically charged, causing threads to repel (i.e., stand up from the surface) so the fabric feels softer and makes it fluffier.
- Anionic softeners and antistatic agents:
  - Salts of monoesters and diesters of phosphoric acid and fatty alcohols.
  - Often used together with conventional cationic softeners.
  - Cationic softeners are incompatible with anionic surfactants as they combine to form a solid precipitate. This is why they are added in the rinse cycle.
  - Anionic softeners can combine with anionic surfactants directly.
  - Other anionic softeners can be based on smectite clays. (Monolayer clays that swell in water.)
  - Some compounds, such as ethoxylated phosphate esters, have softening, anti-static, and surfactant properties.

Fabric softeners (fabric conditioners)

- **INGREDIENT NAME | FUNCTION**
- Water |Process aid
- Diethyl ester dimethyl ammonium chloride | Softening agent
- Fragrance
- Calcium Chloride | Process aid
- Formic acid Hydrochloric acid | Dye pH modifier pH modifier
- Colorant
- Polydimethylsiloxane | Process aid
- Methylisothiazolinone/ Methylchloroisothiazolinone | Preservative
- Cationic polymer | Structuring agent
- Diethylenetriamine pentaacetate, sodium salt | Chelator

Home made fabric softeners

- **Formulation 1**
  - 1 Cup Hair Conditioner (Contains moisturizers and humectants)
  - 3 Cups Hot Water
  - 1 ½ Cups White Distilled Vinegar (Removes detergent residue and scale.)
- **Formulation 2**
  - White Distilled Vinegar
  - Essential Oil (For fragrance.)
- **Formulation 3**
  - 2 Cups Hot Water
  - 1 Cup Baking Soda (Removes metal ions – water softener.)
  - 1 Cup White Distilled Vinegar

Fabric Softener Dryer Sheets

Ingredients | Purpose (Downy and Bounce)

Dipalmethyl Hydroxyethylammonium Methosulfate | Softening and Antistatic agent

Fatty Acid | Softening Agent

Polyester | Substrate Carrier

Clay | Rheology Modifier

Fragrance

Dyes and Dying

Natural plant dyes

Fabrics used:

- Cotton
- Wool
- Silk

Plant materials used:

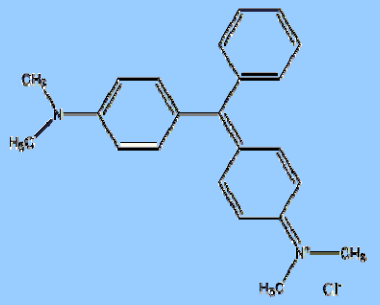
- Onion skins (red and yellow)
- Flowers (as available)
- Coffee
- Tea

Mordants

Common Name	Chemical Name	Use
Alum plus Cream of tartar	Aluminum potassium sulfate Potassium bitartrate	Usually combined in a ratio of 3 parts alum to 1 part cream of tartar
Chrome	potassium dichromate	Used to deepen colors and make them more lasting
Iron (copperas)	Iron(II) sulfate	used as a saddening agent because it makes a color darker or duller
Tin	Tin(II) chloride	used as a brightening agent to make color sharper or lighter
Copper sulfate (blue vitriol)	copper(II) sulfate	used to make colors in the green range as it itself imparts a bluish-green color to fibers
Vinegar	Acetic acid	used to heighten color of a dyebath, especially with reds
Ammonia (non-sudsy, clear)	Ammonia	used to draw colors out of dye materials, especially grasses and lichens

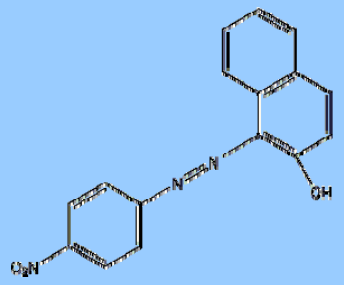
Chemical Dyes

- **Direct dyes**
  - Adhere to fabrics without help from other chemicals. (Mordants optional)



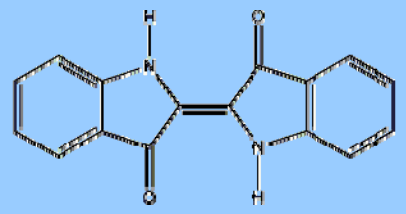
Malachite green

- **Developed dyes**
  - Reaction takes place on the fabric.



Para red

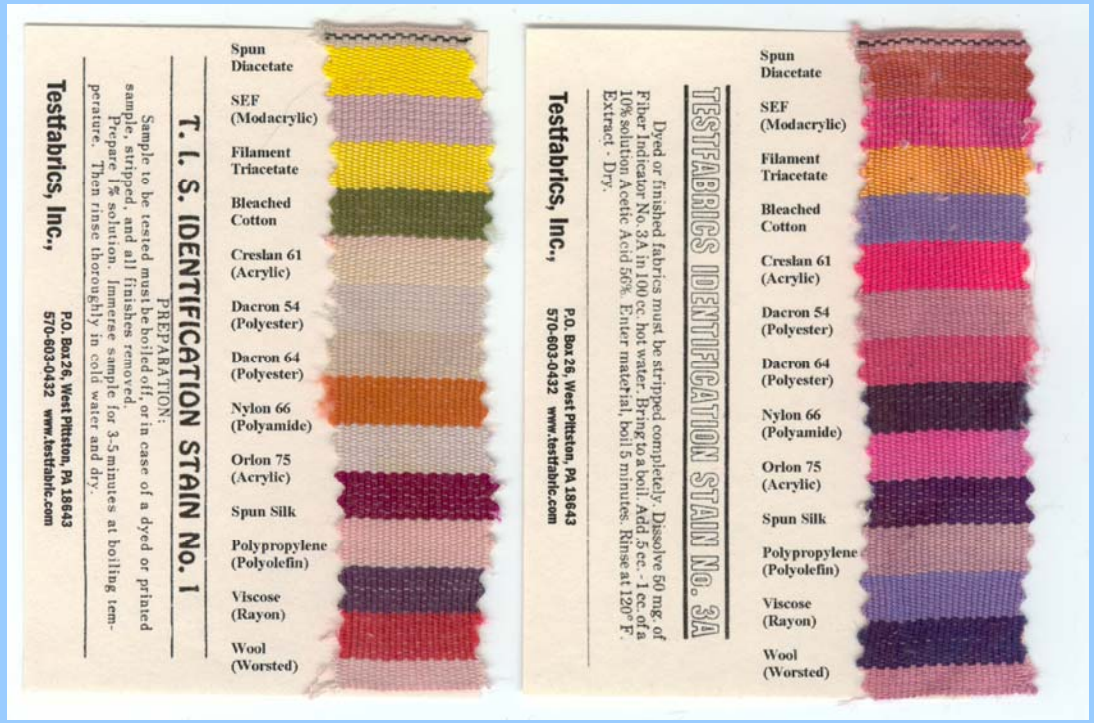
- **Vat dyes**
  - Insoluble dye reduced to a soluble form and applied to the fabric.
  - Air oxidized to colored form.



Indigo

Identification of fabrics

- **T.I.S. Identification Stains** (Testfabrics, Inc.)
  - Mixtures of dyes that color different fabrics differently.
  - Use Multifiber fabrics (Testfabrics, Inc.) as standards.
  - Used in forensics.



Chemistry in the boudoir

Selling sex: cosmetics and personal care products

- Perfumes
- Skin creams
- Tanning and sunscreens

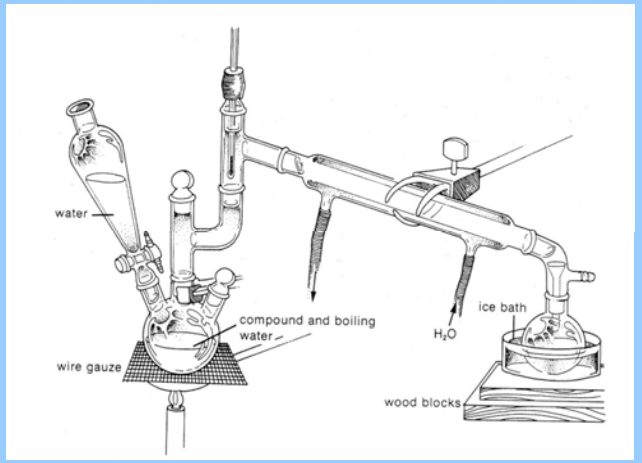
Labs:

- Isolation of an essential oil
- Perfumes
- Preparation of a Skin Cream
- Preparation and Evaluation of Sunscreens

Isolation of an essential oil

Uses 5 g of spices, flowers, herbs or citrus zest

- Original procedure called for extracting the essential oil using methylene chloride.
- Students tended to overheat the extract when they evaporated the methylene chloride.



- Use Jojoba oil. It eliminates additional heating. Only requires some drying with Na_2SO_4 and is ready to use.
- Jojoba oil does not air oxidize and will result in a clear solution. (Alcohol solutions are cloudy.)

Perfumes

Essential oils are classified according to volatility, or the rate they diffuse into the air.

Top notes

Most volatile and are first perceptible odors from a perfume.

Usually of short duration lasting a few minutes to maybe 30 minutes.

Middle notes

Tend to be floral or spicy and give body to blends.

May last for 30 minutes to about an hour.

Base notes

Least volatile

These aromas will last for several hours or longer.

Concentration of perfume oils

Perfume extract (Extrait): 15-40% (IFRA: typical 20%) aromatic compounds (Note: IFRA is the International Fragrance Association)

Eau de Parfum (EdP), Parfum de Toilette (PdT): 10-20% (typical ~15%) aromatic compounds. Sometimes listed as "eau de perfume" or "millésime".

Eau de Toilette (EdT): 5-15% (typical ~10%) aromatic compounds

Eau de Cologne (EdC): Chypre citrus type perfumes with 3-8% (typical ~5%) aromatic compounds

Splash and After shave: 1-3% aromatic compounds

Note: concentrations in % by volume

Classification of notes

Some perfume formulations

Secrets, a spicy blend

Add 4 mL of Jojoba oil or alcohol to a small vial.

Add the following essential oils or fragrance oils:

- ❑ 4 drops allspice oil
- ❑ 2 drops oil of cinnamon
- ❑ 10 drops lavender oil
- ❑ 10 drops rose fragrance oil
- ❑ 4 drops sandalwood

Allure, a floral, soft fragrance (similar to Chanel #5)

Add 6 mL of Jojoba oil or alcohol to a small vial.

Add the following essential oils or fragrance oils:

- ❑ 15 drops of citrus fragance oil
- ❑ 2 drops of rose fragrance oil
- ❑ 10 drops of jasmine fragrance oil
- ❑ 8 drops of lily of the valley fragrance oil
- ❑ 5 drops of floral bouquet fragrance oil
- ❑ 10 drops of sensual fragrance oil

Skin Cream and Sunscreens

Preparation of a skin cream:

Stearic acid
Lanolin
Mineral oil
Triethanolamine
Water

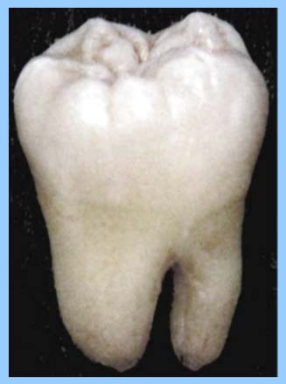
Preparation and Evaluation of Sunscreens

Stearic acid
Glycerin
RG100 silicone elastomer resin gel (Decamethyl cyclopentasiloxane)
Trietanolamine
Water
Cetyl alcohol (1-hexadecanol)
Benzophenone-3 (oxybenzone)
Ethylhexylmethoxycinnamate (octyl methoxycinnamate)

Evaluate with Spectronic 20 to 330 or 340 nm

Chemistry in the boudoir

Toothpaste



Components of toothpaste

Ingredients	% by weight
Humectants	40-70
Water	0-50
Buffers/salts/tartar control	0.5-10
Organic thickeners (gums)	0.4-2
Inorganic thickeners	0-12
Abrasives	10-50
Actives/Antibacterial agent (e.g., triclosan)	0.2-1.5
Surfactants	0.5-2
Flavor and sweetener	0.8-1.5

Fluoride sources provide 1000-15000 ppm fluorine.

Typical toothpaste ingredients

Gums (binding agents)	**Inorganic Thickeners**	**Abrasives**	**Surfactants**	**Humectants**	**Tartar Control Ingredient**
Sodium carboxymethyl cellulose	Silica thickeners	Hydrated silica	Sodium lauryl sulfate	Glycerin	Tetrasodium pyrophosphate
Cellulose ethers	Sodium aluminum silicates	Dicalcium phosphate dihydrate	Sodium N-lauryl sarcosinate	Sorbitol	Gantrez S-70
Xanthan Gum	Clays	Calcium carbonate	Pluronics	Propylene glycol	Sodium tri-polyphosphate
Carrageenans		Sodium bicarbonate		Xylitol	
Sodium alginate		Calcium pyrophosphate	Sodium lauryl sulfoacetate	Polyethylene glycol	
Carbopols		Alumina			

Non-active ingredients include:

Sodium benzoate or ethylparaben: preservatives to prevent growth of micro-organisms.

Sodium saccharine: gives the toothpaste a sweet taste.

Titanium dioxide: coloring agent. It makes the toothpaste opaque and gives it a white color.

Artificial dyes: to make colored toothpastes such as blue, green or red.

Moh's hardness of Dental Abrasives

Compound (Formula)	Moh's Hardness
Talc (For reference)	1
Dentin	3.0-4.0
Tooth enamel	5.0
Baking soda, $NaHCO_3$	2.5
Dicalcium phosphate dihydrate, $CaHPO_4 \cdot 2H_2O$	2.5
Calcium carbonate, $CaCO_3$	3.0
Anhydrous dicalcium phosphate, $CaHPO_4$	3.5
Hydrated silica dioxide, SiO_2	2.5-5.0
Calcium pyrophosphate, $Ca_2P_2O_7$	5.0
Alumina, Al_2O_3	9.25
Diamond (For reference)	10

Making Toothpaste

1. Baking soda and salt.
   - Mix with glycerin.
   - Thin with some water.
   - No flavoring, detergent, or dyes used.
2. Baking soda, salt, and calcium carbonate.
3. Baking soda, salt, calcium carbonate, and detergent (sodium lauryl sulfate).

Testing Toothpaste

- Use commercial and home-made toothpaste.
- Egg shells best approximate tooth enamel.
  - Stain with food color, coffee, tea, and artificially colored drinks
- Test for:
  - Abrasiveness
  - Spreadability
  - pH
  - Foaming ability
  - Cleaning ability
  - Cost analysis

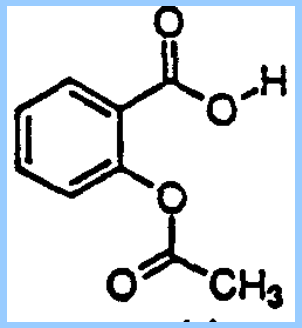
Chemistry in the medicine cabinet

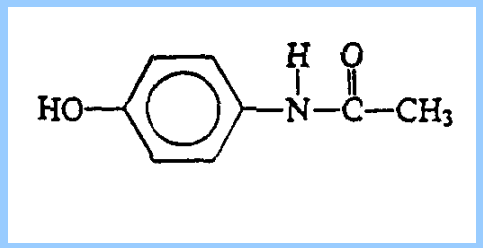
Aches, pains, and pills

Over the counter medications

The Drug Lab:

Synthesis of Aspirin and Acetaminophen





Standardization of a Basic Solution and Analysis of Stomach Antacid Tablets

Other course requirements

- **Take-home exams or worksheets**
- **Complete laboratory report sheets and answer all questions**
- **Write two reports:**

  5 pages double spaced (minimum)

  Minimum of 3 references

  Proper bibliography

  Topics:

  CHM 121:

  1. Some current issue related to chemistry

  2. A consumer product

  CHM 125: Two unrelated consumer products

Course syllabi and experiments can be found at

http://www.chymist.com

On the left-hand menu, click on
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