# Novel Cosmetic Surfactant Systems

**Cosmetic Formulation** 

Perry Romanowski Element 44 Inc. May 3, 2015

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# Perry Romanowski

- Element 44 Inc.
- Brains Publishing Inc.
- Cosmetic Chemist
  - Formulator
  - Inventor
- Writer
- Instructor
- Professional Blogger





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#### Why Teens Don't Need Wrinkle Creams

by LEFT BRAIN on June 26, 2011 - 3 Comments

Cathy's question ... My face is really gross at the moment. My cheeks are flaming with weird red blotchy bumps that I can't seem to get rid of! It's not acne! I've been using Guinot anti-redness treatment but it doesn't seem like its working these bumps

are really worrying me. Also I have some small faint delicate multi-wrinkles up there are there any wrinkle cream suitable for 16 years old? I don't want to be 60 and none of the wrinkle creams would work on me cause when I was little I was so accustomed to heavy creams.

#### The Left Brain Replies:

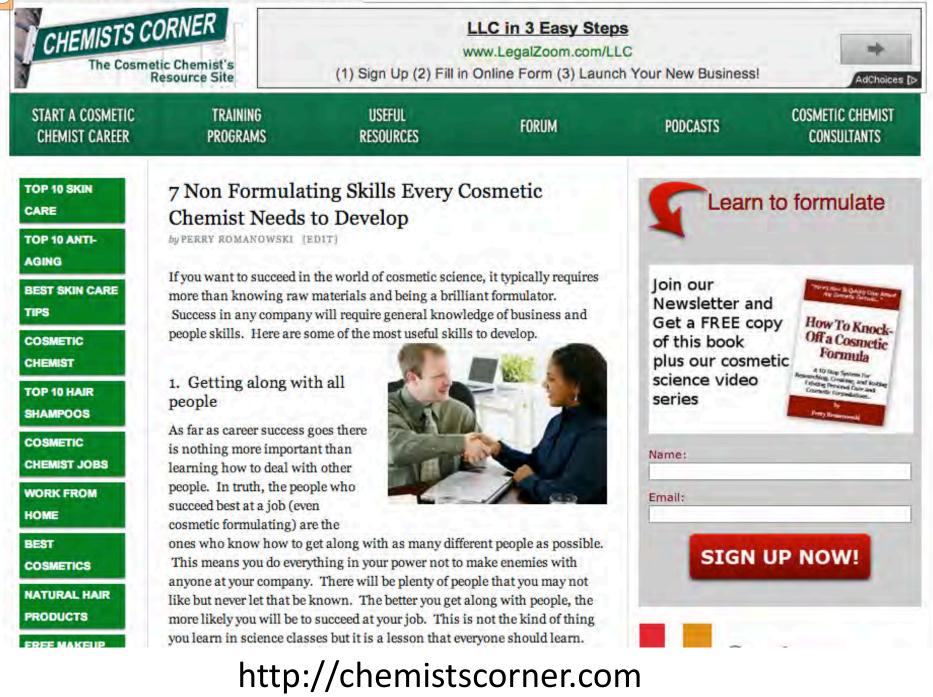
Cathy, I don't know what's causing your blotchy skin bumps, but it sounds like you should see a dermatologist. As far as wrinkles are concerned, I wouldn't be

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### http://thebeautybrains.com









I comment Started by FormulatorSamples October 10 Skin Care products

### **Cosmetic Science Forum**

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From The Cosmetic Chemist' Resource Site

Go

All Discussions	My Bookmarks 🛛	My Discussions 92
Welcome to the F	CLEIN .	w PerryR October 2 General
How to use the fo		
the second second	comments Most recent by	PerryR May 3 General
Supposedly "bett	er" emulsions	
2 comments Most rece	ent by PerryR 8:00AM Co	osmetic Industry
What paraben-fr	ee and formaldehid	le releaser-free conservative to use?
3 comments Most rece	ent by Duncan 3:24AM S	ikin Care products
Substitution of S	LES and SLS	
10 comments Most re-	cent by Duncan 3:16AM	Cosmetic Science talk
Tanning beds inc	rease melanoma in	young women
3 comments Most rece	ent by Duncan 3:07AM C	Cosmetic Industry
Water based hair	/scalp tonic – still i	need an emulsifier
3 comments Most rece	ent by dess October 11	Hair Care products
Formulate Differe	ently	
4 comments Most rece	ent by Eliza October 11	Innovation
Natural? Organic	? Weigh-in please.	
3 comments Most rece	ent by Eliza October 11	Cosmetic Science talk
Natural/Organic	Preservative for too	othpaste

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Start a New Discussion

BOOKINAI KEU DISCUSSIONS
Water based hair/scalp tonic - still
need an emulsifier
3 October 11 dess
Testing of handmade soaps,
anhydrous products and products

containing more than 35% ethanol

**Deel/marked** Discussions

# PRACTICAL COSMETIC FORMULATING

HOME PRE-MODULES

MODULES

RESOURCES

CAREER

BONUS MATERIAL

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free bonuses, just click here.

### Modules

### **Course Description**

Practical Cosmetic Formulation is designed to introduce the student to the principles of cosmetic science and formulation, including: understanding cosmetic form and function, the basics of cosmetic chemistry, cosmetic terminology and techniques, the product development process, formulation of specific cosmetics, an understanding of raw materials and their use, cosmetic product testing, product scale-up and government regulations affecting cosmetics and the consumer.

#### **Course Frequency**

New lessons will be published every other week. A Q&A session will be held monthly.

### Modules

If you want to get up to speed on the basic Math. Biology, and Chemistry you will need to

http://chemistscorner.com/members

#### NAVIGATION

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# Contact

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Facebook

# Objectives

- Learn about cosmetic technologies
- Understand the raw materials used
- Learn the different formulation forms
- Cover specific formulations
  - Cleaning products
  - Moisturizing products

# Agenda

- 9:00 9:30 Introduction to cosmetics
- 9:30 10:30 Cosmetic ingredients
- 10:30 10:45 Break
- 10:45 11:45
- 11:45 12:30
- **Cosmetic formulations**
- 30 Formulation process

# My mission







### Educate

### Inspire

### Entertain

# Cosmetics

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# Purposes of Cosmetics

Improve your...

- Appearence
- Skin Feel
- Odor

# What are Cosmetics?

Articles intended to be rubbed, poured, sprinkled or sprayed on or introduced into or otherwise applied to the human body or any part thereof for cleansing, beautifying, or promoting the attractiveness , or altering the appearance, and articles intended for use as a component of any such articles; except that such term shall not include soap

-FDA CFR

# Color Cosmetics

 $\bigcirc$ 



# Hair Products





# Perfume & Fragrances

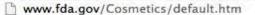
# Oral care Products

### Cosmetics aren't drugs

### Drugs = Treat disease

### Cosmetics = Improve appearance

Can't interfere with metabolism



U.S. Department of Health & Human Services



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### Cosmetics

Home O Cosmetics



Temporary Tattoos May Put You at Risk Think they're just harmless fun? Think again.

#### 1 2 3

#### **Navigate the Cosmetics Section**

Cosmetic Labeling & Label Claims What cosmetic labels can say and what they must say; what label claims mean

Guidance, Compliance & Regulatory Information Resources on legal, regulatory, enforcement, and policy issues related to cosmetics

International Activities

News & Events What's new, meetings & workshops

Product and Ingredient Safety Information on cosmetic products, ingredients, testing, recall policy, and more

Resources for You At-a-plance menus for consumers industry and more

#### Spotlight

- Cosmetics Q&A
- Voluntary Cosmetic Registration Program (VCRP)

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- Color Additives and Cosmetics
- Cosmetic Labeling Manual
- Imports & Exports

#### **Recalls & Alerts**

- Cosmetics Warning Letters
- FDA Recall Policy for Cosmetics

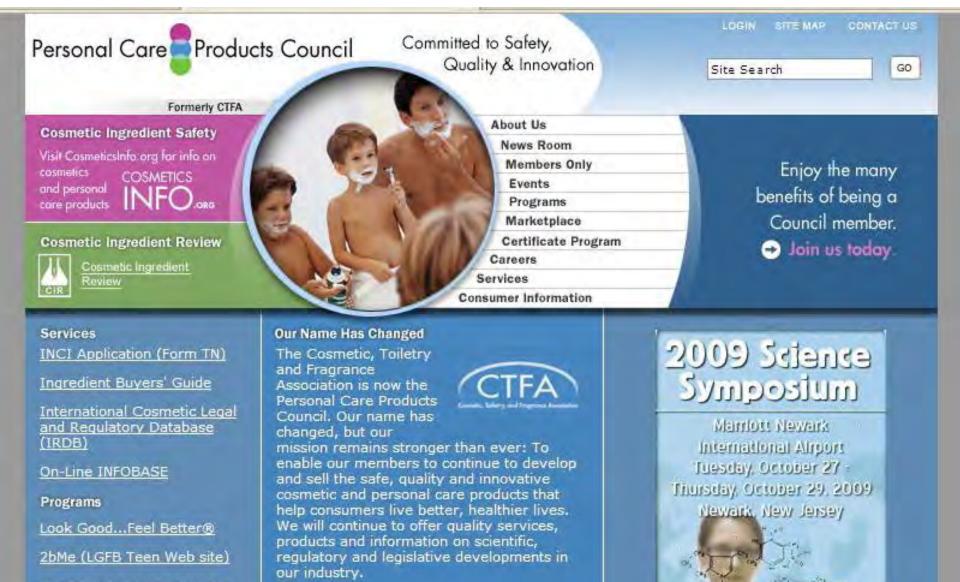
#### **Top Picks**

Preparation for International

http://www.fda.gov/Cosmetics

### $\bigcirc$

### Personal Care Products Council



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SUPPLIERS DIRECTORY

Find the products and services you need.

# International Regulatory bodies

- European Commission
- Health Canada
- Ministry of Health (Japan)
- Department of Health & Ageing (Australia)
- CFDA China



# General Problems addressed by cosmetics

- Appearance
- Feel
- Smell



# Top 10 skin problems

- 1. Dry itchy skin
- 2. Wrinkles
- 3. Acne
- 4. Sagging Skin
- 5. Age spots
- 6. Skin lightening
- 7. Tattoo removal
- 8. Eczema / Dermatitis
- 9. Psoriasis
- 10. Cellulite



# Top 10 hair problems

- 1. Hair Loss
- 2. Unwanted Hair
- 3. Gray Hair
- 4. Hair color change
- 5. Hair feels bad
- 6. Frizzy, unruly hair
- 7. Thinning hair
- 8. Lack of volume
- 9. Shine
- 10. Time needed to style



# Strategies for Improving Appearance

- Remove dirt from surface
  - Cleansing products
- Change the surface

   Exfoliating products
- Leave color behind
   Make-up
- Change color of surface
   Self tanning products



# Strategies for Improving Feel

- Materials that make skin & hair feel better
   Oils and emollients
- Water attracting compounds
  - Moisturizers
- Conditioning products
  - Film forming material

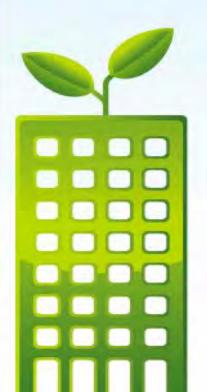


# Strategies for Improving Odor

- Clean odor materials off body
- Cover odors with fragrance
- Kill microbes that cause odor



# Lots of interest in Natural Formulating



# Greenwashing

# Natural has no legal definition

# Natural Standards Groups



# Major US Natural Standards Groups

- USDA
- National Sanitation Foundation
- National Product Association
- OASIS





# International Natural Standards



# **COSMOS** Standards

- Promote organic agriculture
- Use natural resources
- Clean processing and manufacture
- "Precautionary Principle"
- Integrate Green Chemistry principles



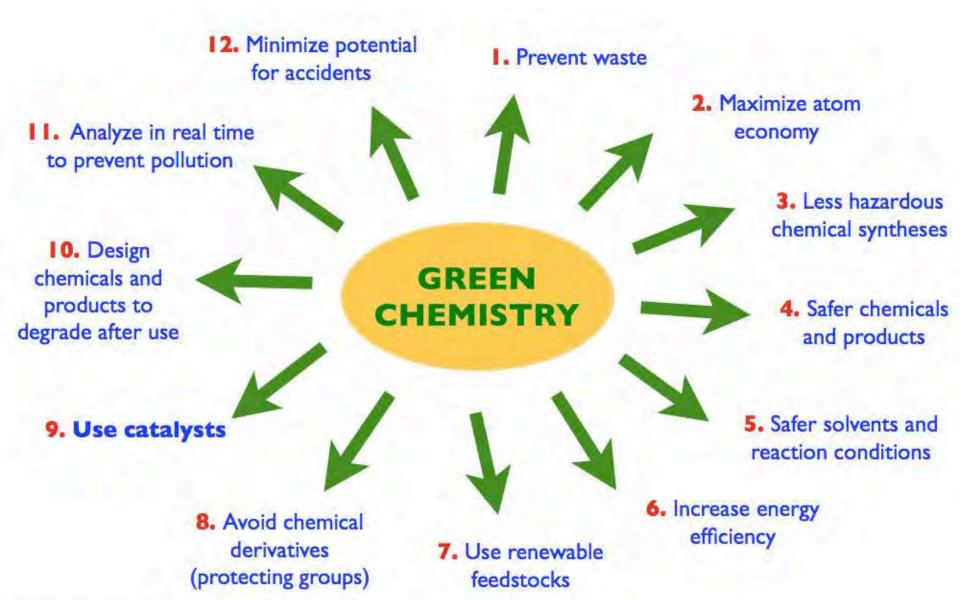








#### **Principles of Green Chemistry**



Anastas and Warner (1998)

## **Basic Definition of Natural**

- Not Synthetically Derived or Synthetically processed
- If it's not from a plant, it's not natural
- USDA definition
- Other standards are not as strict



## **Common Standards**

- Water is natural
- Mineral ingredients are natural
- Physically processed agromaterials are natural
- Some chemical processing of agro materials
- Some synthetics allowed



# Some Prohibited Ingredients

- Parabens
- Formaldehyde Donors
- Petrolatum & petroleum derived
- Propylene glycols
- Sodium Lauryl Sulfate
- Ethanolamines
- Synthetic Silicones
- Synthetic Fragrances
- Synthetic Polymers
- EDTA



# Some Chemistry Allowed

- Distillation
- Esterification & Etherification
- Expression
- Extraction
- Fat Splitting
- Fermentation
- Hydrogenation
- Protein Hydrolysis
- Saponification
- Sulfation (no SLS)



#### **Cosmetic Science Quiz**

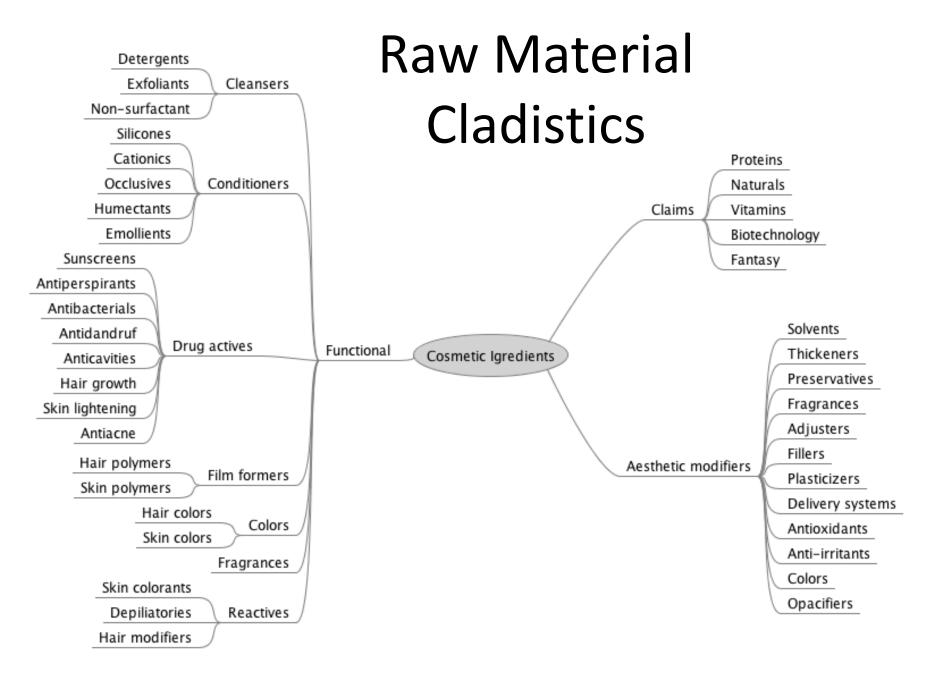
- Which ingredient is not in the top 10 most vilified cosmetic ingredients?
  - 1. Methyl Paraben
  - 2. Mineral Oil
  - 3. Titanium Dioxide
  - 4. Sodium Laureth Sulfate

#### Most Vilified Ingredients on the Internet

Sulfates – SLS / SLES Parabens Talc Petrolatum Mineral Oil **Propylene Glycol** DEA Formaldehyde Aluminum Fragrance



#### **Cosmetic Raw Materials**



#### **Cosmetic Raw Materials**

Functional – Provide the product benefit

 Aesthetic – Improve the aesthetics of the functional ingredients

Claims – Included to help sell the product

## **Functional Raw Materials**

- Ingredients that make cosmetics work
- Cleansers
- Conditioners
- Film formers
- Drug actives
- Reactants
- Colorants
- Fragrances

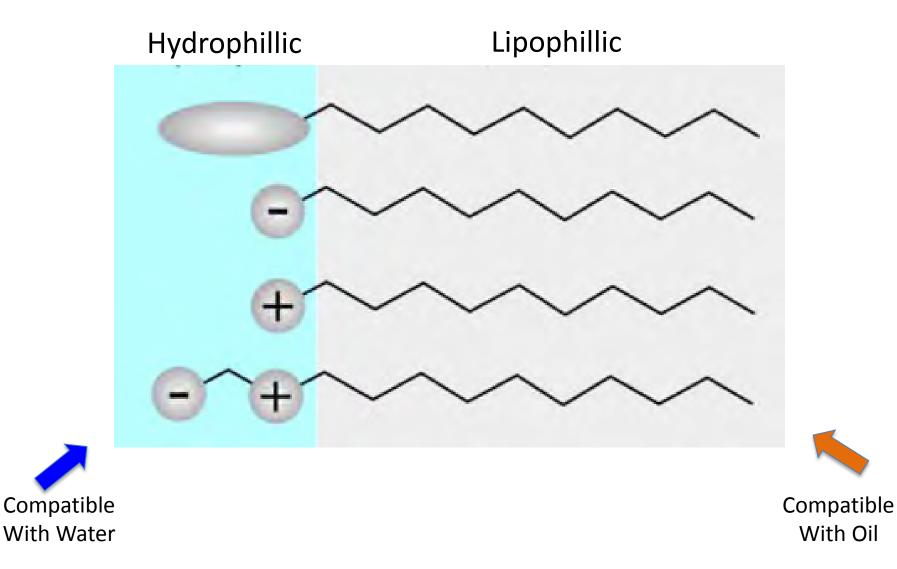


#### Cleansers

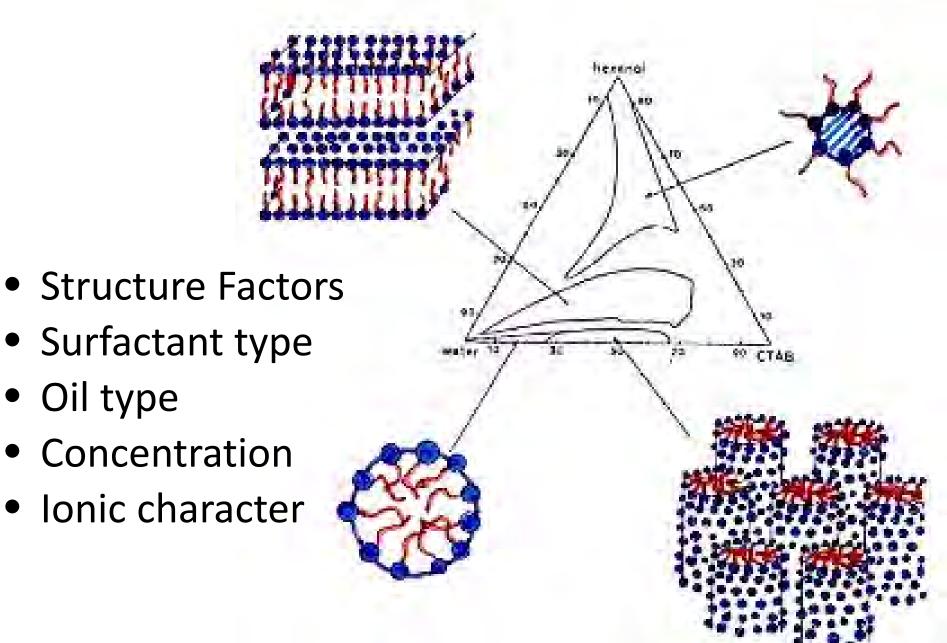
- Ingredients that remove surface dirt / oil
- Some oil based cleansers
- Surfactants



#### Surfactants



#### Surfactant Structures

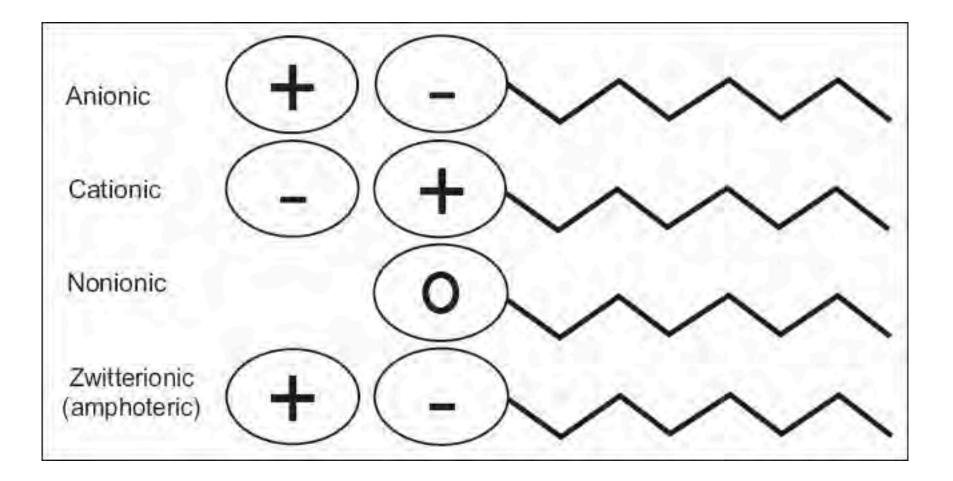


## **Surfactant Functions**

- Cosmetic Benefits
  - Cleaning / Detergency
  - Conditioning
  - Foaming
- Aesthetic benefits
  - Emulsification
  - Wetting / Dispersing
  - Thickening
  - Penetration enhancement
  - Antimicrobial activity
  - Opacification



### **Types of Surfactants**



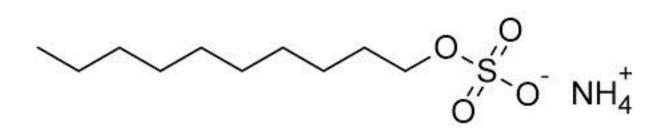
## Anionic Surfactants

- These are the primary cleansing surfactants
- Alkyl Sulfates

– Examples – SLS and ALS

• Alkyl Ether Sulfates - Ethoxylated

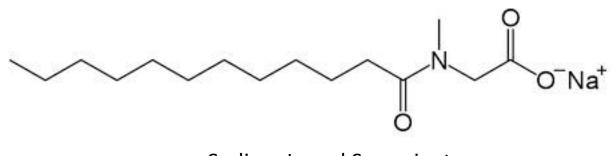
Example – SLES and ALES



## Anionic Surfactants

- Other types
  - Sulfosuccinates
  - Alkylbenzene
     Sulfonates
  - Acyl Methyltaurates
  - Acyl Sarcosinates

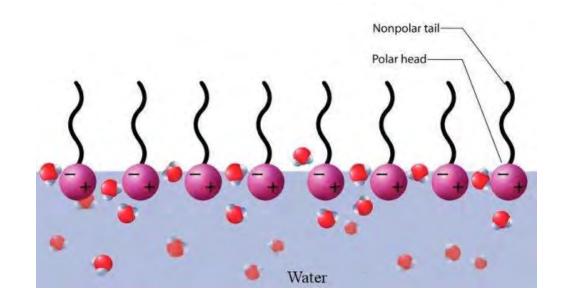
- Acyl Isethionates
- Acyl Polypeptide Condensates
- Monoglyceride Sulfates
- Fatty Glyceryl Ether
   Sulfonates



Sodium Lauryl Sarcosinate

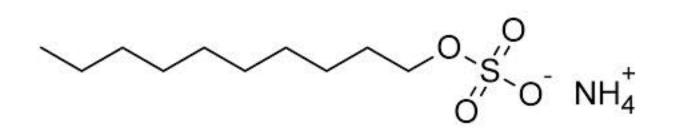
# Anionics

- Why use them?
  - Excellent detergency
  - Relatively inexpensive
  - Good foaming
  - Highly stable
- Drawbacks
  - Can be irritating
  - Drying to hair



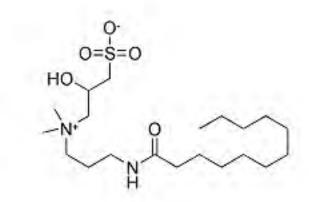
## Sulfates and Naturals

- Unacceptable for cleansing surfactants for natural products
  - Sulfosuccinates
  - Sulfonates
  - Alkyl sulfates



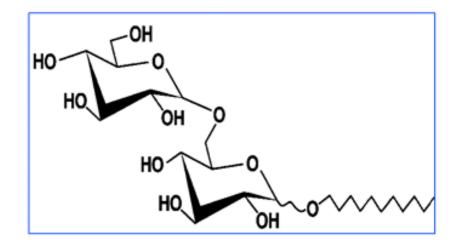
# What is used instead

- Sultaines
  - Mild secondary surfactant, more stable and better viscosity builder
    - e.g. Cocamidopropyl Hydroxysultaine
- Acyl Sarcosinates
  - High foaming secondary surfactant
    - e.g. Sodium Lauryl Sarcosinate



## Natural Surfactant Options

- Alkyl Polyglucoside
  - Natural primary surfactant derived from coconut and sugar
  - Does not build viscosity as well
  - Does not foam as well
  - Higher cost
  - e.g. Lauryl Glucoside

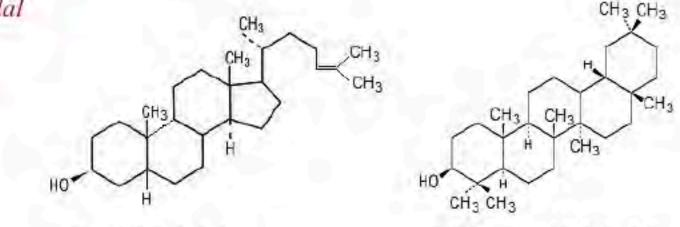


# **Saponin Glycosides**

Parts of plants containing saponins are used as detergents. For example; Root of Saponaria officinalis

#### Types:

Aglycone may be of two types; Steroidal Tri terpenoidal

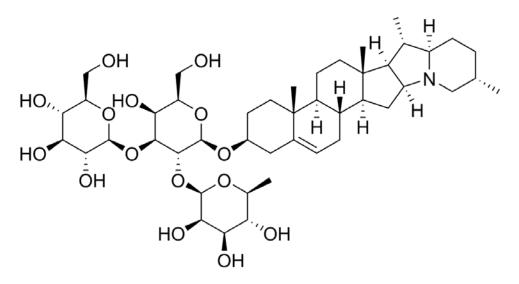


Steroidal skeleton

Tri-terpenoidal skeleton

# Natural Cleansing Surfactants

- Saponins Cleansing Surfactants
- Source: plants marine derived
  - Quillaja saponaria Molina
- Difficult to purify
- Too expensive
- Not as effective
- ~40% less foam
- Highly colored



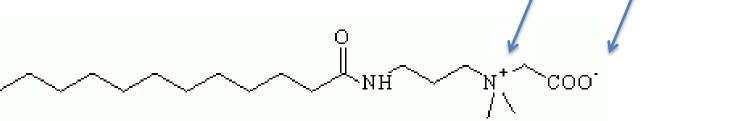
## **Commercially Available Saponins**

- Bio-Saponins (Bio-Botanica)
  - mix of Sarsparilla, Wild Yam, Quillaja and Yucca extracts.
- Neo Actipone Soap Nutshell (Symrise)
   Soap Nut tree (*Sapindus Mukurossi*) extract.
- Andean QD Ultra & Ultra Organic (Desert King)
   Chilean soap bark tree (*Quillaja Saponaria Molina*) extract.

### **Amphoteric Surfactants**

- Can have a positive or negative charge depending on the pH of the solution
  - Zwitterionic
- Types
  - Cocamidopropyl Betaine





Positive

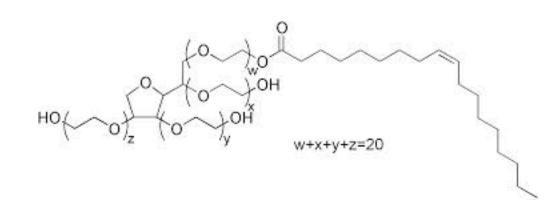
Negative

## **Amphoteric Surfactants**

- Why use them?
  - Good Detergency
  - Less Irritating than anionics
  - Helps thicken system
  - Helps improve foam
- Drawbacks
  - More expensive
  - Do not foam well enough on their own

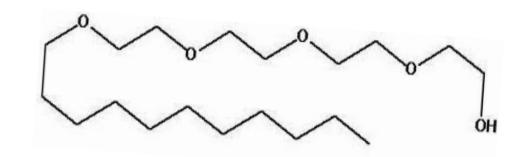
# Non Ionic Surfactants

- Surfactant molecules with no charge
- Types
  - Fatty Alcohol
  - Fatty amines
    - Lauramide DEA
  - Amine Oxides
    - Lauramine Oxide
  - Polysorbates



# Non Ionic Surfactants

- Why use them?
  - Foam enhancer
  - Reduce irritation
  - Conditioning effect
  - Solubilize fragrances
  - Emulsifiers



- Gentle Cleansers
  - PEG-80 Sorbitan Laurate
- Drawbacks
  - More expensive
  - Do not foam well on their own

#### Functional Raw Materials Conditioners & Moisturizers



#### Functional Raw Materials Conditioners & Moisturizers

- Defined
  - Ingredients that improve condition of hair or skin
  - Must be substantive to work

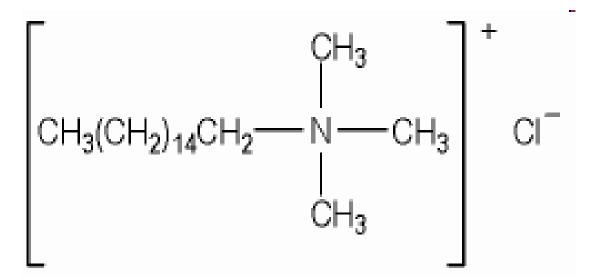
# **Moisturizing Ingredients**

- Quats
- Cationic Polymers
- Silicones
- Occlusives
- Humectants
- Emollients



### Quats

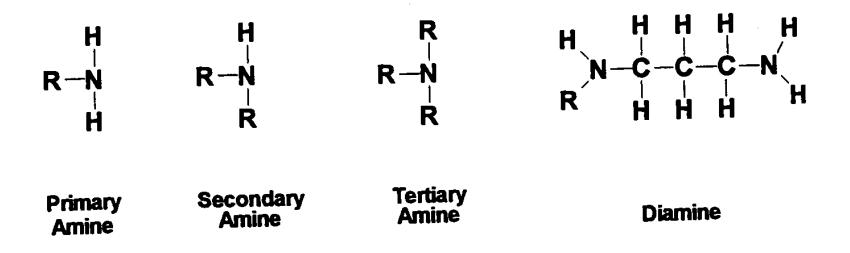
- Cationic Surfactants
  - Hydrophobic tail
  - Hydrophilic head



Cetrimonium Chloride

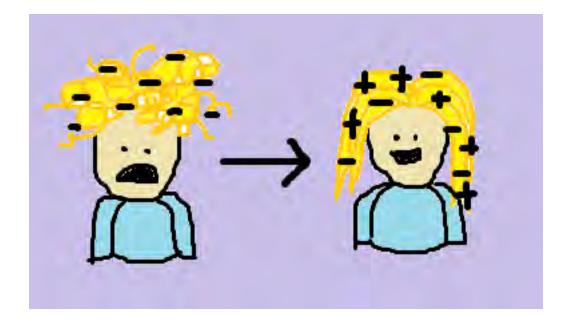
### Quats

- Examples
  - Cetrimonium Chloride
  - Stearalkonium Chloride
  - Dicetyldimonium Chloride
  - Behentrimonium Chloride



### Quats

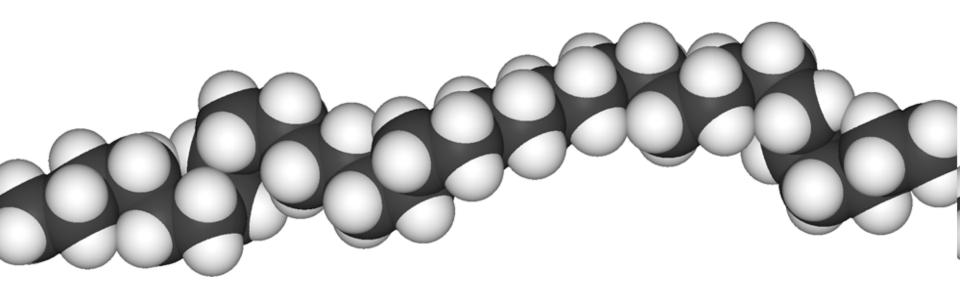
- How do they work?
  - Electrostatic Attraction
  - More damage = more substantivity
  - Longer chain length = more conditioning



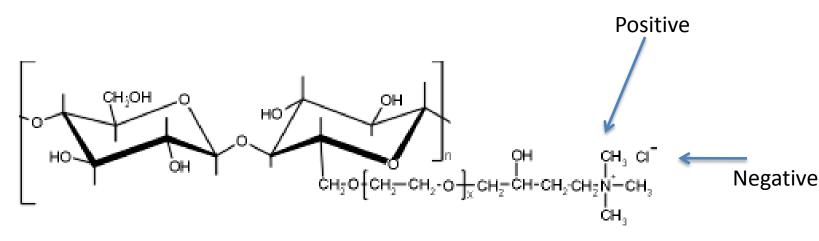
## Quats

- Benefits
  - Effective
  - Easy to work with
  - Less expensive
- Drawbacks
  - Can be irritating
  - Not compatible with anionics
- % Used if formula
  - Up to 5%

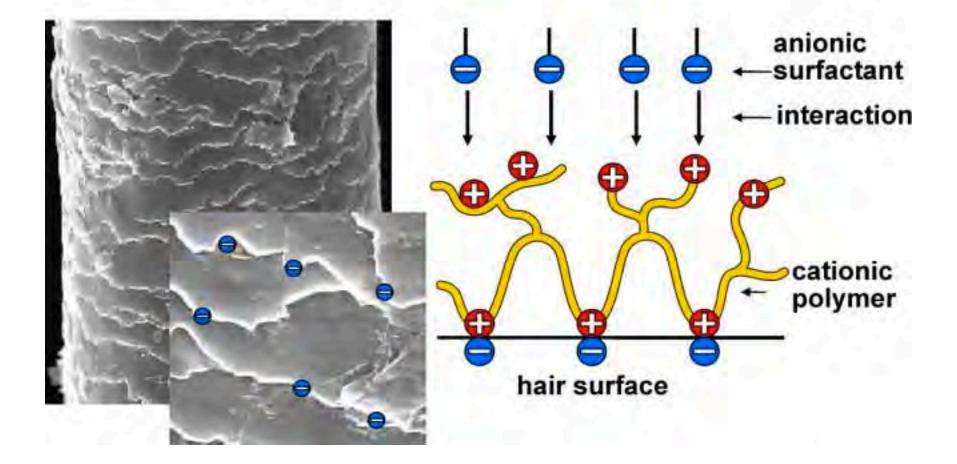
• Large molecules with multiple, positively charged sites



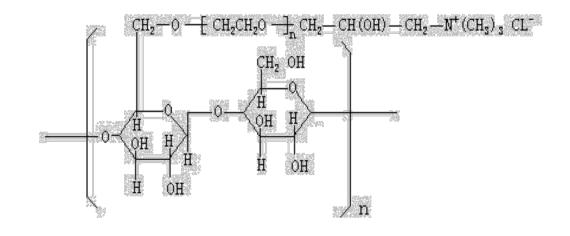
- Common Examples
  - Polyquaternium 4
  - Polyquaternium 7
  - Polyquaternium 10
  - Guar Hydroxypropyltrimonium Chloride



#### Figure 1: Hair structure with cuticula Polymer - Distribution of charge



- Benefits
  - Effective at low levels
  - Compatible with anionics
- Drawbacks
   Can build-up
- % Used if formula
   Up to 5%
  - Usually 1% or less

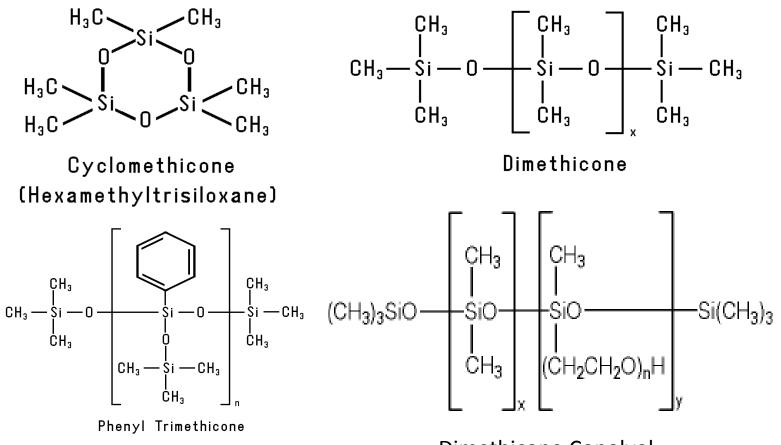


#### Silicones

• Compounds containing silicone



#### Varieties of Silicones



**Dimethicone Copolyol** 

## Silicones

- Benefits
  - Increased shine
  - Increased lubricity
  - Works on undamaged hair
  - Synergistic with cationics
- Drawbacks
  - Build-up
  - Weigh down hair
- % Used if formula
   Up to 2%

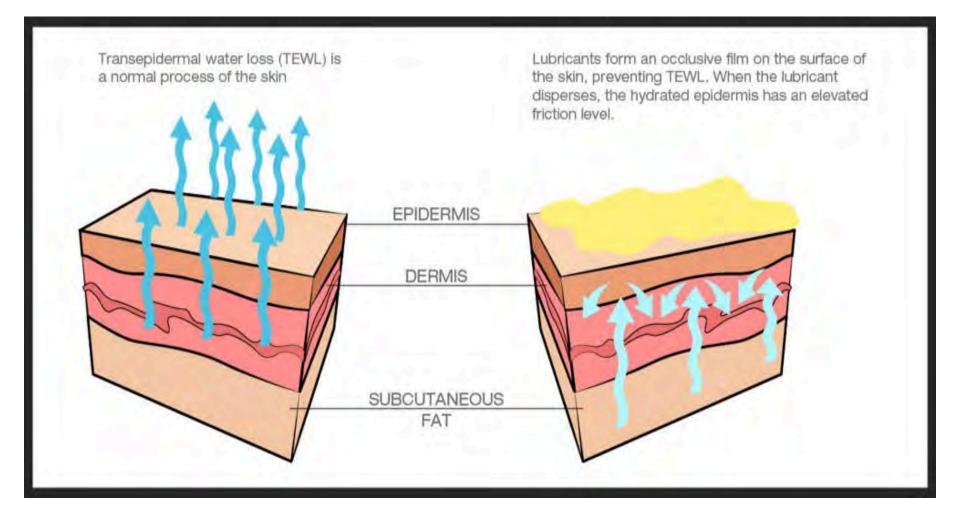


#### Humectants

- Ingredients that attract water
- Usually water soluble
  - Glycerin
  - Propylene Glycol
  - Sorbitol
  - Types of proteins
- Use level
  - 0.5% 15.0%

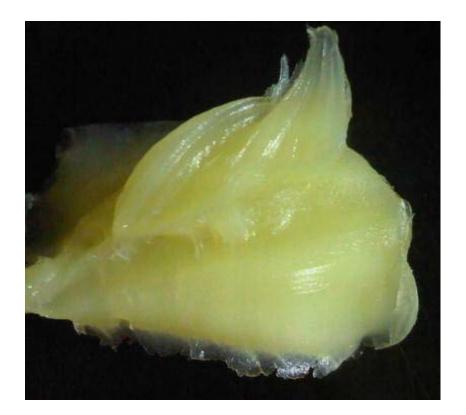
CH<sub>2</sub>OH CHOH CH<sub>2</sub>OH

#### How Occlusives Work

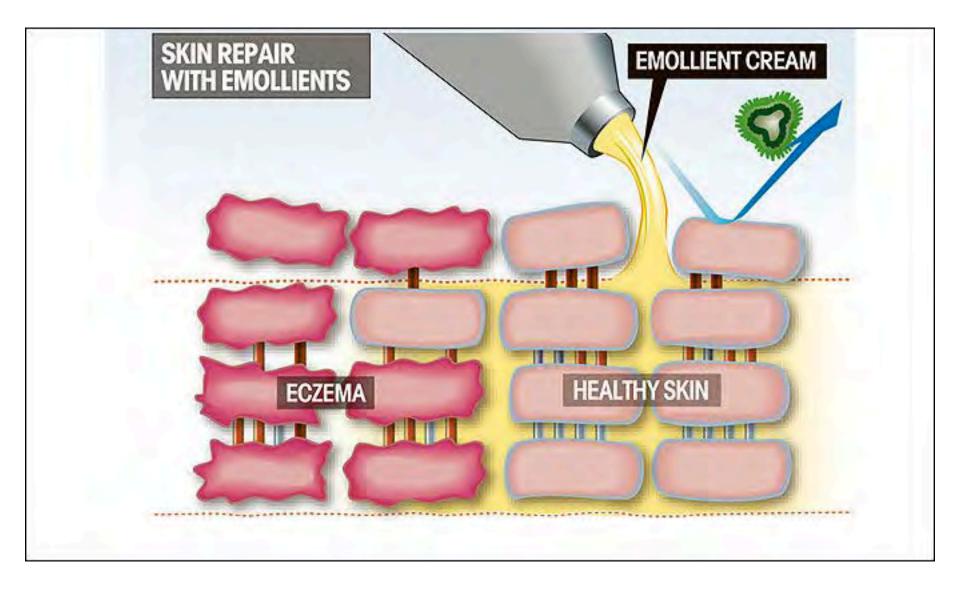


## **Occlusive Agents**

- Water-insoluble materials
- Examples
  - Petrolatum
  - Mineral Oil
  - Dimethicone
- Use Level
  - 5% to 70%

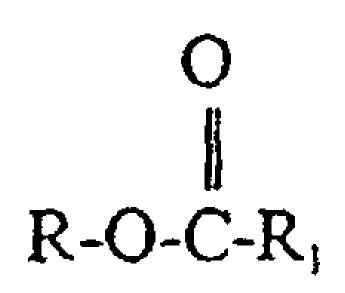


#### Emollients



## Emollients

- Light coating on skin
- Used to improve feel
- Examples
  - Coconut oils
  - Almond oil
  - Esters
  - Silicones
- Use level
  - 5% 25%



#### Functional Ingredients Cosmetic Colorants



## **Cosmetic Colorants**

- Pigments / Dyes
  - Provide color & shine
  - Color formulations
- Two main types
  - Mineral pigments
  - Organic pigments
- Limited by regulations
- Strictly controlled by FDA



Functional Raw Materials Active Ingredients

- Proven to have an effect on cells or fight disease
- Classified as OTC Drugs
  - FDA Monograph
  - In US & elsewhere



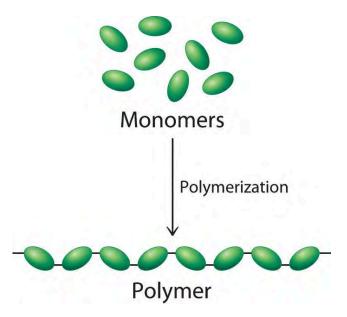
## OTC "cosmetic" Active Ingredients

- Sunscreens
- Anti-acne
- Anti-perspirants
- Anti-dandruff
- Anti-cavity
- Anti-fungal
- Anti-microbial
- Hair growth
- Skin bleaching
- Wart Remover



#### Functional Raw Materials Film Forming Polymers

- Polymers Long chain molecules made up of repeating unit molecules (monomers)
- Wide range of uses
  - Thickeners
  - Conditioning / moisturizers
  - Hair colors
  - Styling polymers



## Functional Raw Materials Reactive Ingredients

- Ingredients that chemically react to produce an effect
- Hair colorants
- Relaxers
- Perms
- Sunless Tanners
- Depilatories



## **Cosmetic Chemistry Quiz**

Which ingredient is NOT something you could possibly find in a cosmetic?

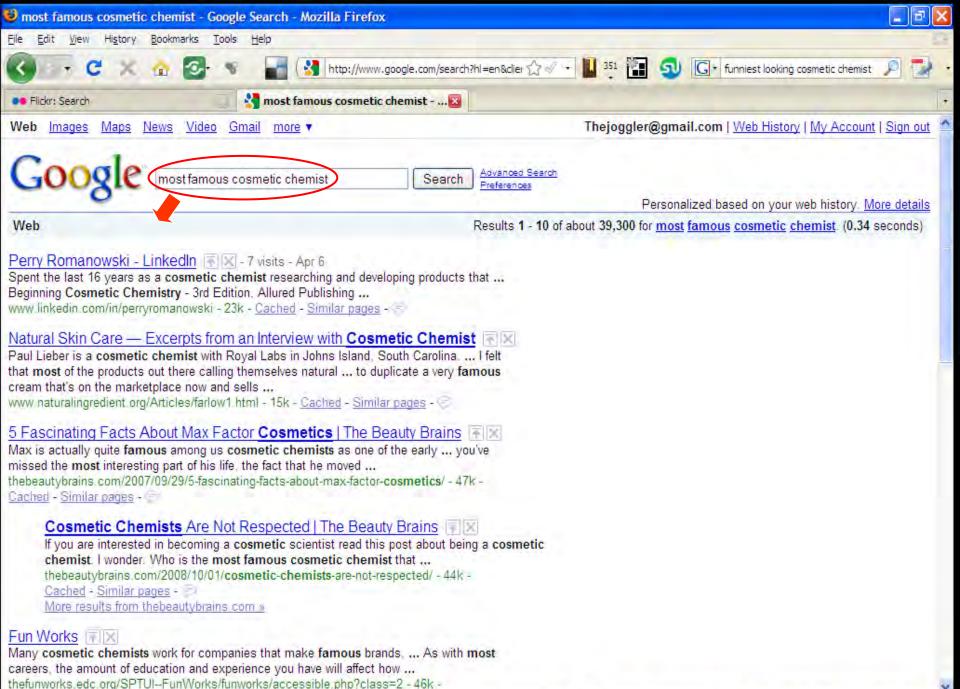
•Whale Vomit

•Sheep placenta

Cow bone marrow

•Bull Semen

#### Break



Open Notebook

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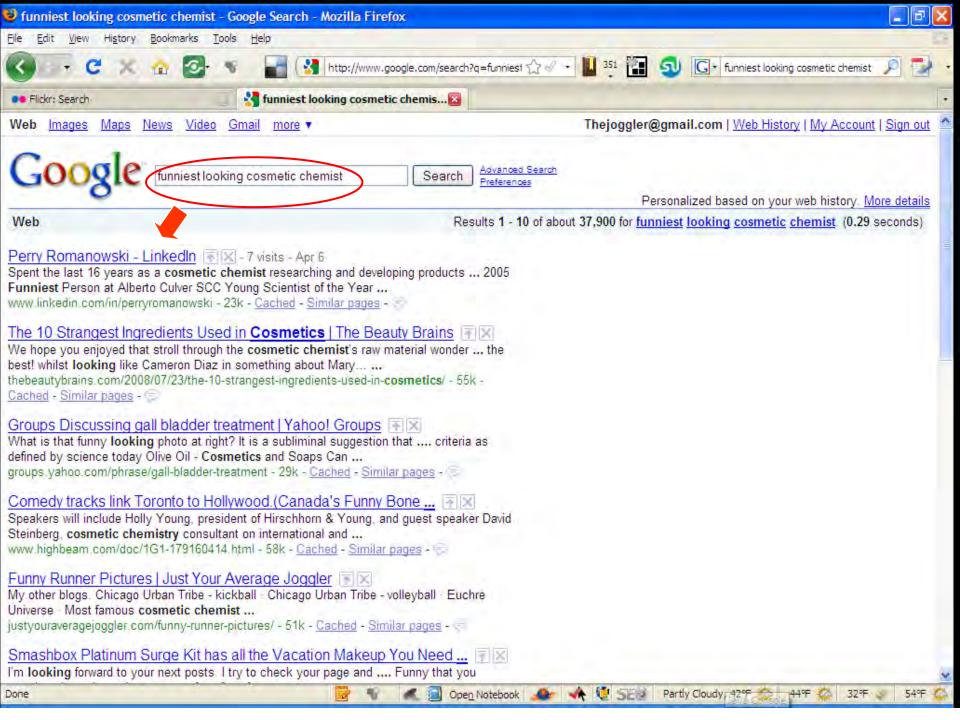
SEG

Partly Cloudy, J

Java Console

Done

32°F



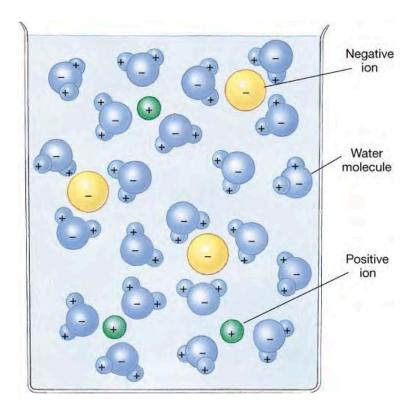
## Aesthetic Raw Materials

- Solvents
- Emulsifiers
- Adjusters
- Preservatives
- Thickeners
- Fragrance
- Fillers
- Delivery Systems



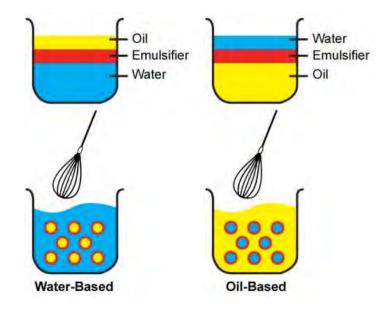
# Solvents

- Ingredients that dilute functional ingredients
- Aid in delivery
- Low cost
- Non-reactive / Compatible
- Most common
  - Water
  - Alcohol
  - Mineral Oil
  - Propylene Glycol



## Emulsifiers

- Ingredients that create oil & water mixtures
- Basis for all creams & lotions
- Emulsions consist of
  - Internal phase
  - External phase
  - Emulsifier
- Very few natural emulsifiers



#### Standard Emulsifiers to Avoid for Natural products

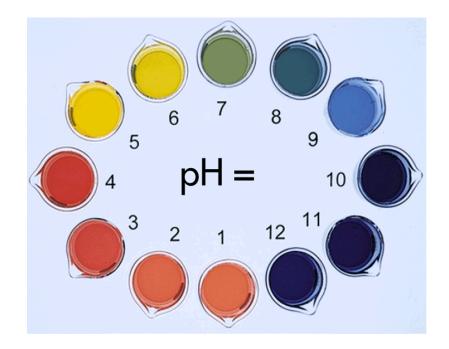
Туре	INCI Name	Reason to exclude
Anionic	Triethanolamine Stearate (Also known as TEA Stearate)	TEA (stearic acid may be animal derived)
	Potassium Cetyl Phosphate	Phosphate content
Nonionic	PEG-100 Stearate	Ethoxylated
	Ceteareth-20	Ethoxylated
	Steareth-2	Ethoxylated
	Bis-PEG/PPG-14/14 Dimethicone	Silicone & PEG based
	Polyacrylate-13	Synthetic polymer
Cationic	Palmitamidopropyl- trimonium chloride	Quaternary

## Natural Emulsifiers – What To Use

- Esters glyceryl caprylate
- Lecithin
  - Challenging to formulate with
- Beeswax/Borate combination
  - Heavy/greasy/unstable
- Soaps
- Saponins
- Polysorbates

# **Formulation Aids**

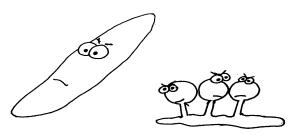
- Ingredients that adjust formulation properties
  - pH
  - Viscosity
  - Solubilizers
- Acids, bases or salts
- Chelating agents
- Nonionic surfactants



#### Preservatives

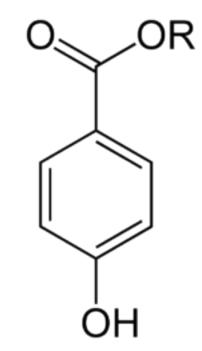
- Compounds that prevent contamination
  - Bacteria
  - Molds
  - Psuedomonas
- Sources of contamination
  - Equipment
  - Ingredients
  - Post-manufacture
  - Consumer





## **Cosmetic Preservatives**

- Parabens
  - Propylparaben
  - Ethylparaben
  - Methylparaben
- Formaldehyde donors
- Phenol derivatives
  - Phenoxyethanol
- Quats
- Alcohol
- Organic compounds
  - Methylchloroisothiazolinone



## "Natural" Preservatives

- Benzoic acid
- Boraxitrus seed extracts
- Copper salts
- Fragrance oils
- Glycerin
- Hinokitiol
- Honey
- Japanese Honeysuckle extracts
- Melaleucol (Tea Tree) oil

- Perillic acid
- Salicylic acid
- Salt
- Silver Chloride
- Sodium Gluconate
- Sorbic acid
- Sugar
- Usnic acid
- Wasabi extract
- Zinc Salts

#### Aesthetic Raw Materials

• Thickeners – Ingredients that increase the thickness of a formula



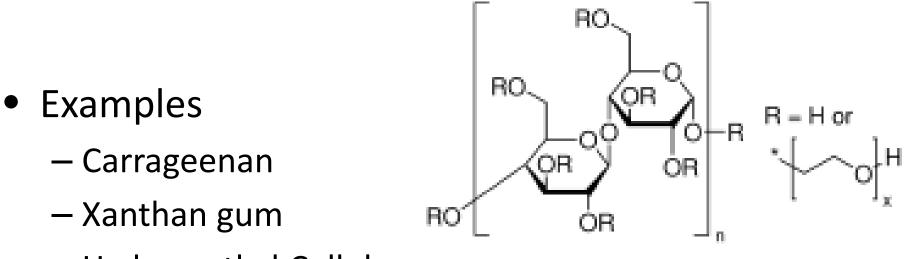
# Lipid Thickeners

- Composed of lipophilic materials
- Solid at room temperature
- Liquid when heated, solid when cooled
- Examples
  - Carnauba wax
  - Cetyl Alcohol
  - Stearyl Alcohol



# **Thickening Technology**

• Cellulose & Carbohydrate thickeners



- Hydroxyethyl Cellulose

#### Cellulose & Carbohydrate thickeners

- How they work
  - Absorb water
  - Internal hydrogen bonding
- Benefits / drawbacks
  - High viscosity
  - Good spreadability
  - Sticky, stringy, cloudy

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- Formula use %
  - Low levels to prevent stickiness
  - 1% or less

Xanthan Gum

CH<sub>2</sub>OH

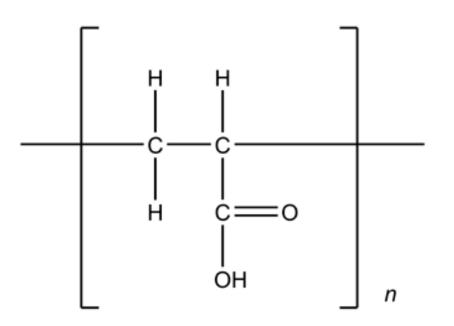
# Mineral Thickeners

- Mined ingredients that hold water
- Different feeling formula
- Can be used to thicken non-aqueous formulas

- Examples
  - Silica
  - Bentonite
  - Magnesium Aluminum Silicate

# Acrylic Thickeners

- Acrylate thickeners
- Examples
  - Carbomer



Acrylic acid monomer unit in carbomer polymers.

#### **Carbomer Thickeners**

- How they work
- Polymer freely moves in solution (Acidic)
- pH is neutralized
   TEA or AMP
- Cross-linking bonds



#### Fragrances

- Used to improve the odor of formula / surface
- Blend of aromatic compounds.
  - Essential oils / naturals
  - Synthetics
- Creation requires art and science



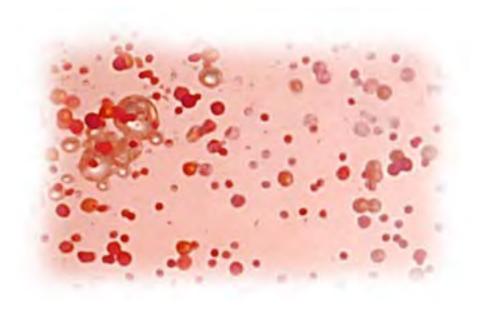
# Fillers

- Used to extend colors
- Choice based on cost & formula needs
- Examples
  - Talc
  - Mica
  - Kaolin
  - Bismuth oxychloride
  - Calcium Carbonate



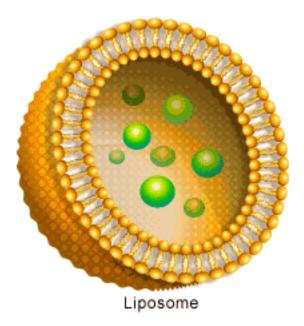
#### **Appearance Modifiers**

- Pearling Agents Opacify formula
- Suspended beads
- Texture modifiers



# **Delivery Systems**

- Ingredients used to better deliver functional ingredients to skin & hair
- Cyclodextrins
- Matrix Polymers
- Liposomes



### Marketing Ingredients

- Added to support a marketing story
- Generally have some functionality
- High concentrations are too expensive
- Give a measure of differentiation
- Recognizable by consumers
  - Positive reception
  - Seem like good ingredients

### Marketing Raw Materials

- Vitamins
- Botanical Extracts
- Proteins
- Anti-Aging
- Used at low levels
- Minimal impact on performance



#### Natural Raw Materials

- Depends on Standards
- Don't expect them to work as well
- They will cost more
- Consumers want products that work



#### **Cosmetic Formulations**



### **Cosmetic Formulation Types**



- Solutions
- Emulsions
- Gels
- Sticks
- Powders
- Aerosols

### Solutions

Simplest formulation Mixture of compounds

#### Examples

- Shampoo
- Skin oils
- Aftershave



# Solution Technology

• Ingredients in Shampoo formulation

- Functional Ingredients 10-20%
  - Cleansing Surfactants
  - Conditioners
- Aesthetic ingredients 80 90%
- Marketing ingredients 0 5%

#### **Example Solution - Shampoo formula**

Shampoo

Water	75.60
Sodium Lauryl Sulfate	12.00
Sodium Laureth Sulfate	5.00
Cocamide DEA	3.00
Hydroxyethylcellulose	0.50
Hydrolyzed Keratin	0.50
Hydroxpropyl Guar Trimonium Chloride	0.20
Sodium Chloride	2.00
DMDM Hydantoin	0.20
Fragrance	1.00
Color	qs

#### Natural - Shampoo

	a farmer of the second s			
	Formula Name			Batch size
	Tier 3 Natural Standard Shampoo			500
	Purpose	INGREDIENT	%	Amt, In Batch
1	Aesthetic – Solvent	Water	42.40	212.00
2	Functional – Conditioning	Guar Hydroxypropyltrimonium Cl	0.300	
3	Aesthetic – pH adjustment	Citric Acid	0.30	1.50
4	Functional – Secondary Surfactant	Cocamidopropyl Betaine	8.00	
5	Functional – Surfactant	Coco Glucoside	15.00	75.00
6	Functional – Surfactant	Decyl Glucoside	20.00	the second
7	Functional – Conditioning	Glycerin	5.00	25.00
8	Aesthetic – Thickener	Polyacrylate 33	5.00	the second s
9	Aesthetic – Opacifier	Glycol Distearate	1.00	
10	Aesthetic – Fragrance	Lavender Oil	0.50	
11	Aesthetic – Preservative	Caprylhydoxamic Acid & Glyceryl Caprylate & Methylpropanediol	1.00	5.00
12	Aesthetic – Thickening	Sodium Chloride	1.50	7.50
		TOTAL	100.000	500.00
	Procedure:		Specificati	ons
	1. Begin mixing item #1 in container. Begin	heating to 70C		
	<ol> <li>Add items #2 - #7</li> <li>At 70C add item #9. Mix for 10 min &amp; coo</li> </ol>	4		5.0 - 5.5 4000 - 7000
	4. At 40C add items #10, 11 and 12		Viscosity -	4000 - 7000
A	5. At <30C mix 10 – 15 min	line -		
	6. Check pH and viscosity. Adjust as require	ed		

#### Natural Body Wash

Ingredient	Function	Wt, %
Sodium Coco Sulfate	Primary Surfactant	10.4
Coco Glucoside	Secondary surfactant	15.4
Lauryl Glucoside	Secondary surfactant	4
Xanthan Gum	Thickener	1.6
Apple Juice	Marketing ingredient	3
Sodium Benzoate	Preservative	0.5
Citric Acid	pH adjustment	QS
Sodium Chloride	Viscosity adjustment	QS
Fragrance	Fragrance	QS
Water	Carrier	QS to 100

\* Meets NaTrue Standard

### Emulsions

Mix of Oil & Water Held together with Emulsifier

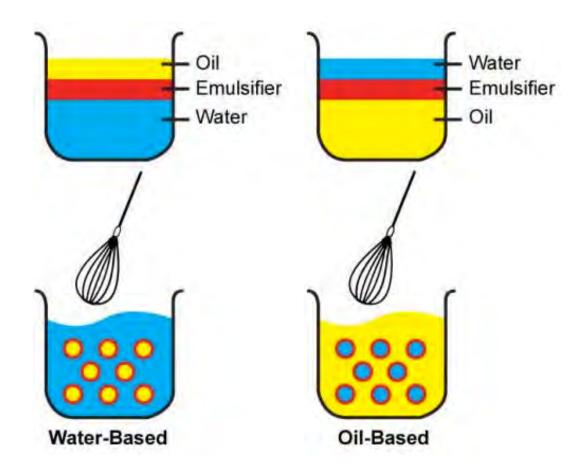
Examples

- Lotions
- Conditioners
- Moisturizers



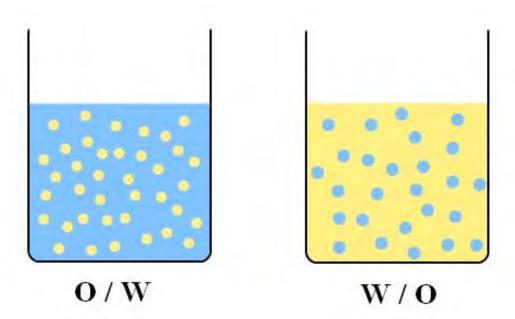
#### **Emulsions Components**

- Internal phase
  - Discontinuous phase
- External phase
  - Continuous
     phase
- Emulsifier



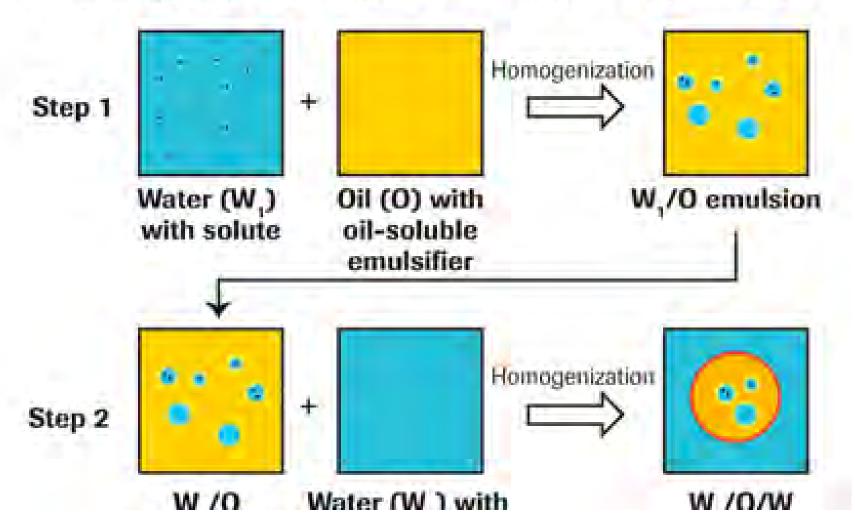
### **Emulsions Types**

- Configuration
  - Oil in Water (O/W)
  - Water in Oil (W/O)
  - Multiple emulsions (W/O/W)



#### **Multiple Emulsions**

#### **Two Steps of Multiple Emulsion Preparation**



#### **Emulsions Particles**

- Classified by particle size
  - Solutions <5 nm</p>
  - Micelles 5 10 nm
  - Microemulsions 10 100 nm
    - Clear
    - Stable
  - Macroemulsions >100nm
    - Opaque
    - Unstable

#### **Emulsions Particles**

- Particle size is determined by
  - Amount of agitation
  - Temperature
  - Component concentration
  - Type of emulsifier and oil
- Generally, smaller particles are more stable

#### **General Moisturizing Cream**

- Functional ingredients 10 50%
- Aesthetic ingredients 50 90%
- Marketing ingredients 0 5%

- Oil in Water emulsion O/W
- Water in oil emulsion W/O

# Creating a formula

- Pick oil phase
- Pick appropriate emulsifier
   HLB method for choosing
- Decide on formula structure
  - O/W less greasy but less effective
  - W/O more effective, more expensive

#### Moisturizing Cream Formula

	Formula Name			Batch size	
	Moisturizing Cream	Oil in Water		500	grams
				Amt. In	
	Purpose	INGREDIENT	%	Batch	Phase
1	Diluent	Water	79.650	398.25	w
2	Thickener	Carbomer (2%)	5.000	25.00	W
3	Humectant	Glycerin	3.000	15.00	w
4	Preservative	Methylparaben	0.100	0.50	w
5	Neutralizer	Triethanolamine	0.900	4.50	w
6	Coemulsifier	Cetyl Alcohol	2.000	10.00	0
7	Emulsifier	Stearic Acid	0.800	4.00	0
8	Emulsifier	Glyceryl Stearate SE	1.500	7.50	0
9	Preservative	Propylparaben	0.050	0.25	0
10	Occlusive	Isopropyl Myristate	1.500	7.50	0
11	Occlusive	Mineral oil	5.000	25.00	0
12	Fragrance	Fragrance	0.500	2.50	m
		TOTAL	100.000	500.00	
	Procedure:		Specificatio	ns	
	1. Begin mixing item #1 in cont	ainer. Heat to 75C			
	2. Add items #2 thru #5	4. 11-11-750		5.0 - 5.5	
	<ol> <li>Separately mix items #6 - #1</li> <li>Slowly mix oil phase with water</li> </ol>	1. Heat to 75C	VISCOSITy =	15,000 - 20,	000 cps
	5. Mix for 30 min and begin cod				
	6. At <40C add item #12	ing to 200			
	7. Check pH and viscosity.				
				1	

### Natural Body Lotion

Ingredient	Function	%
Water	Diluent	QS to 100
Glycerin	Humectant	3
Sodium Stearoyl Glutamate	Emulsifier	0.5
Dehydroacetic Acid (and) Benzyl Alcohol	Preservative	0.8
Xanthan Gum	Thickener	1.0
Cetearyl Alcohol	Emulsifier	2
Polyglyceryl-2 Dipolyhydroxystearate	Secondary emulsifier	2
Glyceryl Stearate	Secondary emulsifier	1
Dicaprylyl Ether	Emollient	5
Oleyl Erucate	Emollient	2
Olive Oil (Organic certified)	Emollient	5

# Gel formula

• Thickened solution or emulsion



# Types of Gel

- Styling Gels
  - Normal Hold
  - Extra Hold
- Shaving gel
- Hand gels



### Gel formulas

• Ingredients in gel formulas

- Functional Ingredients 10-30%
  - Styling Polymers
  - Conditioning Ingredients
- Aesthetic ingredients 70 90%
- Marketing ingredients 0 5%

#### **Example Styling Gel**

	Formula Name			Batch size	
	Normal Gel			500	grams
				Amt. In	
	Purpose	INGREDIENT	%	Batch	Phase
1	Solvent	Water	72.180	360.90	а
2	Thickener	Carbomer	0.500	2.50	а
3	Adjustment Agent	Disodium EDTA	0.200	1.00	а
4	Humectant	Glycerin	0.500	2.50	а
5	Stabilizer	Benzophenone-4	0.020	0.10	а
6	Preservative	Dazolidinyl urea & iodopropynyl butylcarbamate	0.100	0.50	а
7	Solvent	Water	20.000	100.00	b
8	Styling polymer	PVP K-90	2.000	10.00	b
9	Styling polymer	PVP/dimethylaminoethylmethacrylate copolymer	3.000	15.00	b
10	Solubilizer	Oleth-20	0.800	4.00	b
11	Fragrance	Fragrance	0.200	1.00	b
12	Neutralizer	Aminomethylpropanol	0.500	2.50	b
		TOTAL	100.000	500.00	
	Procedure:		Specificatio	ns	
	1. Begin mixing item #1 in co				
	<ol><li>Add item #2 slowly to prev</li></ol>	ent clumping		6.0 - 6.2	
	3. Add items #3 - #6		Viscosity =	25,000 - 35,	000
	<ol> <li>In a separate container mi</li> <li>Add items #8 &amp; #9</li> </ol>	IX Item #7			
	6. Premix #10 & #11. Add to	polymer mixture			
	7. Add item #12 and mix until				
		er solution. Mix 30 minutes until clear.			
	9. Take pH and viscosity rea	dings			

#### Natural Styling Gel

	Formula Name			Batch size
	Tier 3 Natural Standard Gel			500
a.	Purpose	INGREDIENT	%	Amt. In Batch
1	Aesthetic – Solvent	Water	90,400	452.00
2	Functional – Conditioning	Sorbitol	2.500	12.50
3	Functional – Conditioning	Glycerin	3.500	17.50
4	Functional - Hold / Thickening	Dehydoxanthan Gum	2.000	10.00
5	Aesthetic – Preservative	Benzyl Alcohol	1.000	5.00
6	Aesthetic – Fragrance	Fragrance	0.200	1.00
7	Functional - Hold	Acacia Gum	0.400	2.00
_		TOTAL	100.000	500.00
	Procedure:		Specifications	5
	1. Begin mixing item #1 in container. Beg	gin heating to 45C		
	2. Add items 2,3, &4			5.5-6.0
_	3. Premix item 5&6. Add to formula		Viscosity = 7	15,000 - 20,000
	4. Cool to 30C. Add item #7			
			and the second second second	A 10 1



#### Cosmetic Chemistry Quiz

Which one is the FAKE beauty gadget?

- Ceramic unipolar magnet that controls acne
- Wand that shoots oxygen into your skin to smooth, tone & stimulate
- Hand held laser that makes your hair grow
- Electronic headband that relaxes muscles to remove wrinkles

#### **Creating Cosmetic Formulas**



#### Sources for Starting Formulas

Patents Books Harry's Cosmeticology **Chemical suppliers** Prospector.com Trade journals Happi.com Colleagues Ingredient lists – LOIs



"Chelators work by binding trace metals like iron, which are needed for survival by microorganisms. In shampoo formulations, they can improve foam and prevent hard water bathroom deposits."

### Getting information from patents

- Google patents
- Sections of patent
- Finding formulas
- Finding testing ideas
- Working around patents

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#### Relevant Parts of a patent

- Title / Abstract
- Background good historical info here
- Summary / Description Good background
- Claims Most important

- Gives details %, ingredients, etc.

• Examples – The formulas, tests

#### Using Ingredient Lists as Starting Formulas

- Look at the LOI of competitive products
- Sources of LOI and claims information
  - http://drugstore.com
  - http://ulta.com
- Use the 1% line exercise to guess at formula

home >	beauty	> skin	care >	lotions >	creams
--------	--------	--------	--------	-----------	--------



#### How to read cosmetic ingredient lists

- Ingredient Labeling
- Legal requirement
- Use standardized names (INCI)
- Proper order
  - In order above 1%
  - Below 1% is mostly arbitrary (colors at the end)

# Ingredient listing tips

- Fragrance is rarely over 1%
- Adjustment ingredients are low
- Natural sounding ingredients are usually below 1%
- Ingredients over 1% are most important in the formula

#### Ingredient list example

- Identify formula type
- Guess the 1% line
- Identify key ingredients, guess at % levels
- Ignore below 1% ingredients in first formula efforts

#### Ingredient list example Skin lotion

Water, Safflower Seed Oil, Glyceryl Stearate, Glycerin, Jojoba Seed Oil, Borage Seed Oil, Cetyl Alcohol, Vitamin E Acetate, Dimethicone, Aloe Vera Gel, Shea Butter, Sodium Ascorbyl Phosphate (Vitamin C), Phenoxyethanol, L Ergothioneine, Ethylhexyl Glycerin

#### **Possible Starting Formula**

• Water	86.0
<ul> <li>Safflower Seed Oil</li> </ul>	5.0
<ul> <li>Glyceryl Stearate</li> </ul>	3.0
<ul> <li>Glycerin</li> </ul>	3.0
<ul> <li>Jojoba Seed Oil</li> </ul>	1.0
<ul> <li>Borage Seed Oil</li> </ul>	1.0
Cetyl Alcohol	1.0
<ul> <li>Preservative</li> </ul>	qs

#### Where is the 1% line?

- Hair Shampoo formula
  - Water, Ammonium Lauryl Sulfate, Ammonium Laureth Sulfate, Sodium Chloride, Cocoamide MEA, Glycol Distearate, Dimethicone, Ammonium Xylenesulfonate, Vanilla Planifolia Fruit Extract, Cocos Nucifera Milk Coconut, Fragrance, Cetyl Alcohol, Polyquaternium-10, Sodium Citrate, Sodium Benzoate, Disodium EDTA, PEG-7M, Citric Acid, Propylene Glycol, Methylchloroisothiazolinone, Methylisothiazolinone, Blue No. 1

#### **Possible Starting Formula**

• Water	77.9
<ul> <li>Ammonium Lauryl Sulfate</li> </ul>	8.0
<ul> <li>Ammonium Laureth Sulfate</li> </ul>	7.0
Sodium Chloride	1.8
<ul> <li>Cocoamide MEA</li> </ul>	1.8
<ul> <li>Glycol Distearate</li> </ul>	1.5
<ul> <li>Dimethicone</li> </ul>	1.0
<ul> <li>Ammonium Xylenesulfonate</li> </ul>	1.0
<ul> <li>Preservative</li> </ul>	qs

#### Where is the 1% line?

- Hair Conditioner formula
  - Water (aqua), Cetearyl Alcohol, Glycerin, Cyclomethicone, Behentrimonium Methosulfate, Behentrimonium Chloride, Cetyl Alcohol, Wheat Germ Oil (triticum vulgare), Hydrolyzed Silk, Panthenol, Tocopheryl Acetate, Jojoba Oil (buxus chinensis), Aloe Barbadensis Leaf Juice, Fragrance, Propylene Glycol, Methylparaben, Propylparaben, Diazolidinyl Urea, Citric Acid, Red 33, Blue 1

#### **Possible Starting Formula**

• Water	87.0
Cetearyl Alcohol	5.0
Glycerin	3.0
Cyclomethicone	2.0
<ul> <li>Behentrimonium Methosulfate</li> </ul>	1.0
<ul> <li>Behentrimonium Chloride</li> </ul>	1.0
Cetyl Alcohol	1.0

#### Use Knock-out Experiments

• Objective: To figure out the function & effect of ingredients in a formulation

- Procedure:
  - Create a series of formulas substituting main solvent for one ingredient
  - Evaluate effect on specification tests, stability, performance

#### Knock-out Example

Form	ula Name: Bubble Bath												
			Control	Test A	Test B	Test C	Test D	Test E	Test F	Test G	Test H	Test I	Test J
	Ingredient	%	Amount										
1	Water	64.50	322.50	324.50	337.5	323.00	387.50	397.5	325.00	332.50	325.00	325.00	325.00
2	Polyquaternium 10	0.40	2.00	-	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
3	Glycerin	3.00	15.00	15.00	-	15.00	15.00	15.00	15.00	15.00	15.00	15.00	15.00
4	Tetrasodium EDTA	0.10	0.50	0.50	0.50	-	0.50	0.50	0.50	0.50	0.50	0.50	0.50
5	Ammonium Lauryl Sulfate (28%)	13.00	65.00	65.00	65.00	65.00	-	65.00	65.00	65.00	65.00	65.00	65.00
6	Ammonium Laureth Sulfate (25%)	15.00	75.00	75.00	75.00	75.00	75.00	-	75.00	75.00	75.00	75.00	75.00
7	PEG 5 Cocamide	0.50	2.50	2.50	2.50	2.50	2.50	2.50	-	2.50	2.50	2.50	2.50
8	Cocamidopropyl Betaine	2.00	10.00	10.00	10.00	10.00	10.00	10.00	10	-	10	10	10.00
9	Citric Acid	0.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	2.50	-	2.50	2.50
10	DMDM Hydantoin	0.20	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	-	2.50
11	Fragrance (Parfum)	0.80	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	4.00	-
	TOTAL	100.000											

#### **Knock-out Experiment shortcuts**

- Ingredients you don't have to knockout
- Dyes
- Feature ingredients
- Preservatives

#### Knock-out Experiment Example 2

For	rmula Name		F	Batch size	
	Intensive Cream	Oil in Water		500	grams
	Purpose	INGREDIENT	%	Amt. In Batch	Phase
1	Diluent	Water	70.470	352.35	W
2	Dye	Blue No 2	0.044	0.22	W
3	Thickener	Carbomer (2%)	5.000	25.00	w
4	Humectant	Glycerin	5.000	25.00	w
5	Preservative	Methylparaben	0.100	0.50	w
6	Neutralizer	Triethanolamine	0.900	4.50	w
7	Coemulsifier	Cetyl Alcohol	2.000	10,00	0
8	Emulsifier	Stearic Acid	0.800	4.00	0
9	Emulsifier	Glyceryl Stearate SE	2.000	10.00	0
10	Preservative	Propylparaben	0.050	0.25	0
11	Occlusive	Petrolatum	3.000	15.00	0
12	Occlusive	Mineral oil	10.000	50.00	0
13	Feature	Silk Protein	0.100	0.50	m
14	Feature	Aloe Vera gel	0.080	0.40	m
15	Fragrance	Fragrance	0.500	2.50	m
		TOTAL	100.044	500.22	

#### Knock-out Experiment Example 2

/	Formula Name																
	Intensive Cream	Oil in Water															
I																	
	Purpose	INGREDIENT	Control	Α	В	С	D	Е	F	G	Н		J	K	L	М	N
1	Diluent	Water	70.426	70.47	75.43			71.33				70.48	73.43				70.93
2	Dye	Blue No 2	0.044	1.1	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
3 ;	: Thickener	Carbomer (2%)	5.000	5.00	-	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
4	Humectant	Glycerin	5.000	5.00	5.00	-	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
5	Preservative	Methylparaben	0.100	0.10	0.10	0.10		0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
6	Neutralizer	Triethanolamine	0.900	0.90	0.90	0.90	0.90		0.90	0.90	0.90	0.90	0.90	0.90	0.90	0.90	0.90
7	Coemulsifier	Cetyl Alcohol	2.000	2.00	2.00	2.00	2.00	2.00		2.00	2.00	2.00	2.00	2.00	2.00	2.00	2.00
8	Emulsifier	Stearic Acid	0.800	0.80	0.80	0.80	0.80	0.80	0.80	•	0.80	0.80	0.80	0.80	0.80	0.80	0.80
9 (	Emulsifier	Glyceryl Stearate SE	2.000	2.00	2.00	2.00	2.00	2.00	2.00	2.00	•	2.00	2.00	2.00	2.00	2.00	2.00
10	Preservative	Propylparaben	0.050	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05		0.05	0.05	0.05	0.05	0.05
11 ;	: Occlusive	Petrolatum	3.000	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	1.1	3.00	3.00	3.00	3.00
12 ;	Occlusive	Mineral oil	10.000	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	10.00	1.1	10.00	10.00	10.00
13	Feature	Silk Protein	0.100	0.10									0.10			0.10	0.10
14	Feature	Aloe Vera gel	0.080	0.08								0.08	0.08				0.08
15	Fragrance	Fragrance	0.500	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	
' <b>ـــــ</b> '	<u> </u>	<u> </u>			ل	ليت	لينت		ل								
		TOTAL	100.000	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
<u> </u>		· · · · · · · · · · · · · · · · · · ·													$ \longrightarrow $		
I		′															

#### 15 batches total

#### **Knock-out Experiment Simplified**

	Formula Name											
	Intensive Cream	Oil in Water										
	Purpose	INGREDIENT	Control	В	С	E	F	G	Н	J	K	N
1	Diluent	Water	70.426	75.43	75.43	71.33	72.43	71.23	72.43	73.43	80.43	
2	Dye	Blue No 2	0.044	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.04
3	Thickener	Carbomer (2%)	5.000	-	5.00	5.00	5.00	5.00	5.00	5.00	5.00	
4	Humectant	Glycerin	5.000	5.00		5.00	5.00	5.00	5.00	5.00	5.00	5.00
5	Preservative	Methylparaben	0.100	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10	0.10
6	Neutralizer	Triethanolamine	0.900	0.90	0.90	-	0.90	0.90	0.90	0.90	0.90	0.90
7	Coemulsifier	Cetyl Alcohol	2.000	2.00	2.00	2.00	-	2.00	2.00	2.00	2.00	2.00
8	Emulsifier	Stearic Acid	0.800	0.80	0.80	0.80	0.80	-	0.80	0.80	0.80	0.80
9	Emulsifier	Glyceryl Stearate SE	2.000	2.00	2.00	2.00	2.00	2.00	-	2.00	2.00	2.00
10	Preservative	Propylparaben	0.050	0.05	0.05	0.05	0.05	0.05	0.05	0.05	0.05	
11	Occlusive	Petrolatum	3.000	3.00		3.00	3.00	3.00	3.00	-	3.00	
12	Occlusive	Mineral oil	10.000	10.00	10.00	10.00	10.00	10.00	10.00	10.00		10.00
13	Feature	Silk Protein	0.100								0.10	
14	Feature	Aloe Vera gel	0.080									
15	Fragrance	Fragrance	0.500	0.50	0.50	0.50	0.50	0.50	0.50	0.50	0.50	-
′												
		TOTAL	100.000	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
′												
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#### 10 batches total

#### Knockout experiment Case Study

- Test a shampoo formula
- See what you can learn from the study
- Things to test
- Specification
  - рН
  - Viscosity
- Performance
  - Foam
  - Conditioning

#### Knockout experiment Case Study

Formula Name		Batch size						
Basic Clear Cleansing Shampoo		500	grams					
INGREDIENT	%	Control	А	В	С	D	Е	F
Water	38.800	194.00	394.00	244.00	209.00	219.00	204.00	199.00
Sodium Laureth Sulfate	40.000	200.00	-	200.00	200.00	200.00	200.00	200.00
Sodium Lauroylmethyltaurate	10.000	50.00	50.00	-	50.00	50.00	50.00	50.00
Cocamide DEA	3.000	15.00	15.00	15.00	-	15.00	15.00	15.00
Glycerin	5.000	25.00	25.00	25.00	25.00	-	25.00	25.00
Sodium Chloride	2.000	10.00	10.00	10.00	10.00	10.00	-	10.00
Fragrance	1.000	5.00	5.00	5.00	5.00	5.00	5.00	-
DMDM Hydantoin	0.200	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Water	0.000	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TOTAL	100.000	500.00	500.00	500.00	500.00	500.00	500.00	500.00
	INGREDIENT Water Sodium Laureth Sulfate Sodium Lauroylmethyltaurate Cocamide DEA Glycerin Sodium Chloride Fragrance DMDM Hydantoin Water	INGREDIENT%Water38.800Sodium Laureth Sulfate40.000Sodium Lauroylmethyltaurate10.000Cocamide DEA3.000Glycerin5.000Sodium Chloride2.000Fragrance1.000DMDM Hydantoin0.200Water0.000	INGREDIENT         %         Control           Water         38.800         194.00           Sodium Laureth Sulfate         40.000         200.00           Sodium Lauroylmethyltaurate         10.000         50.00           Cocamide DEA         3.000         15.00           Glycerin         5.000         25.00           Sodium Chloride         2.000         10.00           Fragrance         1.000         5.00           DMDM Hydantoin         0.200         1.00           Water         0.000         0.00	INGREDIENT         %         Control         A           Water         38.800         194.00         394.00           Sodium Laureth Sulfate         40.000         200.00         -           Sodium Lauroylmethyltaurate         10.000         50.00         50.00           Cocamide DEA         3.000         15.00         15.00           Glycerin         5.000         25.00         25.00           Sodium Chloride         1.000         50.00         10.00           Fragrance         1.000         5.00         5.00           DMDM Hydantoin         0.200         1.00         1.00           Water         0.000         0.00         0.00	INGREDIENT         %         Control         A         B           Water         38.800         194.00         394.00         244.00           Sodium Laureth Sulfate         40.000         200.00         -         200.00           Sodium Laureth Sulfate         10.000         50.00         -         200.00           Sodium Laureth Sulfate         10.000         50.00         -         200.00           Sodium Lauroylmethyltaurate         10.000         50.00         -         200.00           Cocamide DEA         3.000         15.00         15.00         15.00           Glycerin         5.000         25.00         25.00         25.00           Sodium Chloride         2.000         10.00         10.00         10.00           Fragrance         1.000         5.00         5.00         5.00           DMDM Hydantoin         0.200         1.00         1.00         1.00           Water         0.000         0.00         0.00         0.00	INGREDIENT         %         Control         A         B         C           Water         38.800         194.00         394.00         244.00         209.00           Sodium Laureth Sulfate         40.000         200.00         -         200.00         200.00           Sodium Laureth Sulfate         10.000         50.00         -         50.00         200.00           Sodium Lauroylmethyltaurate         10.000         50.00         50.00         -         50.00           Cocamide DEA         3.000         15.00         15.00         15.00         -         Glycerin         5.000         25.00         25.00         25.00         25.00         25.00         25.00         5.00<	INGREDIENT         %         Control         A         B         C         D           Water         38.800         194.00         394.00         244.00         209.00         219.00           Sodium Laureth Sulfate         40.000         200.00         -         200.00         200.00         200.00           Sodium Laureth Sulfate         10.000         50.00         -         50.00         200.00         200.00           Sodium Lauroylmethyltaurate         10.000         50.00         50.00         -         50.00         50.00           Cocamide DEA         3.000         15.00         15.00         15.00         -         15.00           Glycerin         5.000         25.00         25.00         25.00         25.00         -           Sodium Chloride         2.000         10.00         10.00         10.00         10.00         10.00           Fragrance         1.000         5.00         5.00         5.00         5.00         5.00           DMDM Hydantoin         0.200         1.00         0.00         0.00         0.00         0.00           Water         0.000         0.00         0.00         0.00         0.00         0.00	INGREDIENT         %         Control         A         B         C         D         E           Water         38.800         194.00         394.00         244.00         209.00         219.00         204.00           Sodium Laureth Sulfate         40.000         200.00         -         200.00 </td

#### **Knockout Results**

	pH	Viscosity	Foam
Control Formula	5.5	9000	8
Sodium Lauryl Sulfate	6.0	4000	3
Sodium Laurylmethosulfate	5.7	6000	4
Sodium Chloride	5.5	500	8
Cocoamide DEA	4.8	2000	5
Glycerin	5.4	9000	8
Fragrance	5.5	12000	10

# Using Knockout Results

- pH is off...
  - Too high add SLS or SLMS
  - Too low add Cocamide DEA
- Viscosity is off...
  - Too high add fragrance
  - Too low can try SLS, SLMS, Salt, Cocamide DEA
- Foam is off...

– Too low can try SLS, SLMS, Cocamide DEA

# **Knockout Limitations & DOE**

- Limitations
  - Too many batches to make
  - Miss synergistic effects
  - Results in unrealistic results
- DOE Design of Experiment
  - More thorough study
  - Understand synergies between ingredients
  - Not as useful for cosmetics

# **Morning Session Summary**

- Introduction to cosmetics
- Review of cosmetic ingredients
- Review of cosmetic formulation types
- Beginning steps in creating new formulas

• This afternoon will focus on creating more optimal formulations



#### Cosmetics



# Purposes of Cosmetics

Improve your...

- Appearence
- Skin Feel
- Odor

# What are Cosmetics?

Articles intended to be rubbed, poured, sprinkled or sprayed on or introduced into or otherwise applied to the human body or any part thereof for cleansing, beautifying, or promoting the attractiveness , or altering the appearance, and articles intended for use as a component of any such articles; except that such term shall not include soap

-FDA CFR



#### Perfume & Fragrances

# Oral care Products

#### Cosmetics aren't drugs

#### Drugs = Treat disease

#### Cosmetics = Improve appearance

Can't interfere with metabolism

# International Regulatory bodies

- European Commission
- Health Canada
- Ministry of Health (Japan)
- Department of Health & Ageing (Australia)
- CFDA China



#### General Problems addressed by cosmetics

- Appearance
- Feel
- Smell



# Top 10 skin problems

- 1. Dry itchy skin
- 2. Wrinkles
- 3. Acne
- 4. Sagging Skin
- 5. Age spots
- 6. Skin lightening
- 7. Tattoo removal
- 8. Eczema / Dermatitis
- 9. Psoriasis
- 10. Cellulite



#### Strategies for Improving Appearance

- Remove dirt from surface
  - Cleansing products
- Change the surface

   Exfoliating products
- Leave color behind
   Make-up
- Change color of surface
   Self tanning products



# Strategies for Improving Feel

- Materials that make skin & hair feel better
   Oils and emollients
- Water attracting compounds
  - Moisturizers
- Conditioning products
  - Film forming material



# Strategies for Improving Odor

- Clean odor materials off body
- Cover odors with fragrance
- Kill microbes that cause odor



### Greenwashing

#### Natural has no legal definition

#### Major US Natural Standards Groups

- USDA
- National Sanitation Foundation
- National Product Association
- OASIS





#### International Natural Standards



# **COSMOS** Standards

- Promote organic agriculture
- Use natural resources
- Clean processing and manufacture
- "Precautionary Principle"
- Integrate Green Chemistry principles











### **Principles of Green Chemistry**



Anastas and Warner (1998)

## **Common Standards**

- Water is natural
- Mineral ingredients are natural
- Physically processed agromaterials are natural
- Some chemical processing of agro materials
- Some synthetics allowed



# Some Prohibited Ingredients

- Parabens
- Formaldehyde Donors
- Petrolatum & petroleum derived
- Propylene glycols
- Sodium Lauryl Sulfate
- Ethanolamines
- Synthetic Silicones
- Synthetic Fragrances
- Synthetic Polymers
- EDTA



# Some Chemistry Allowed

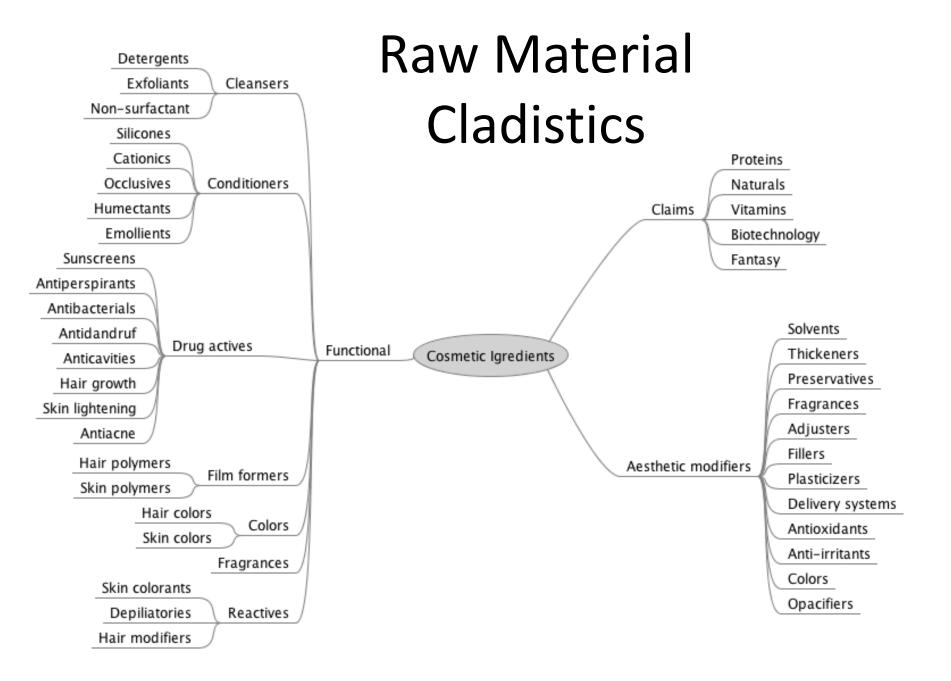
- Distillation
- Esterification & Etherification
- Expression
- Extraction
- Fat Splitting
- Fermentation
- Hydrogenation
- Protein Hydrolysis
- Saponification
- Sulfation (no SLS)



#### **Cosmetic Science Quiz**

- Which ingredient is not in the top 10 most vilified cosmetic ingredients?
  - 1. Methyl Paraben
  - 2. Mineral Oil
  - 3. Titanium Dioxide
  - 4. Sodium Laureth Sulfate

#### **Cosmetic Raw Materials**



#### **Cosmetic Raw Materials**

Functional – Provide the product benefit

 Aesthetic – Improve the aesthetics of the functional ingredients

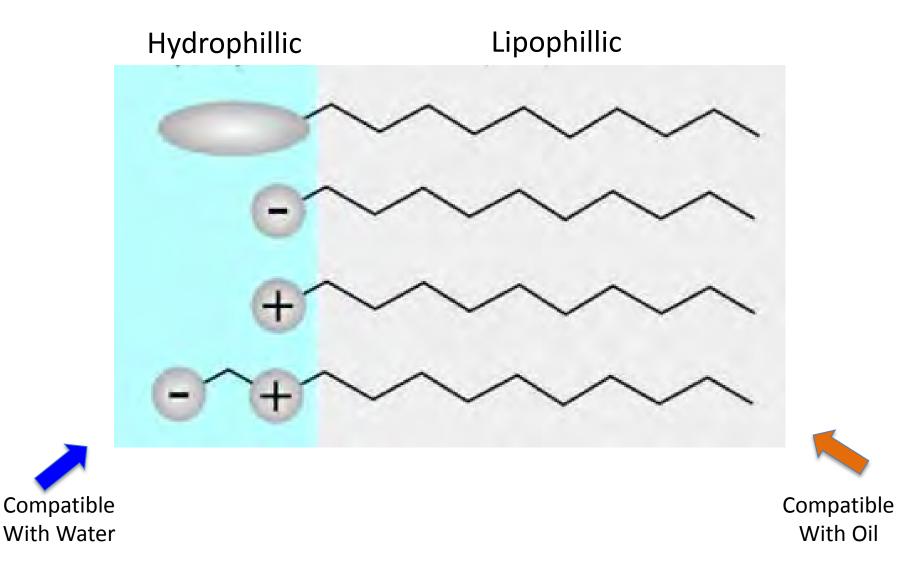
Claims – Included to help sell the product

## **Functional Raw Materials**

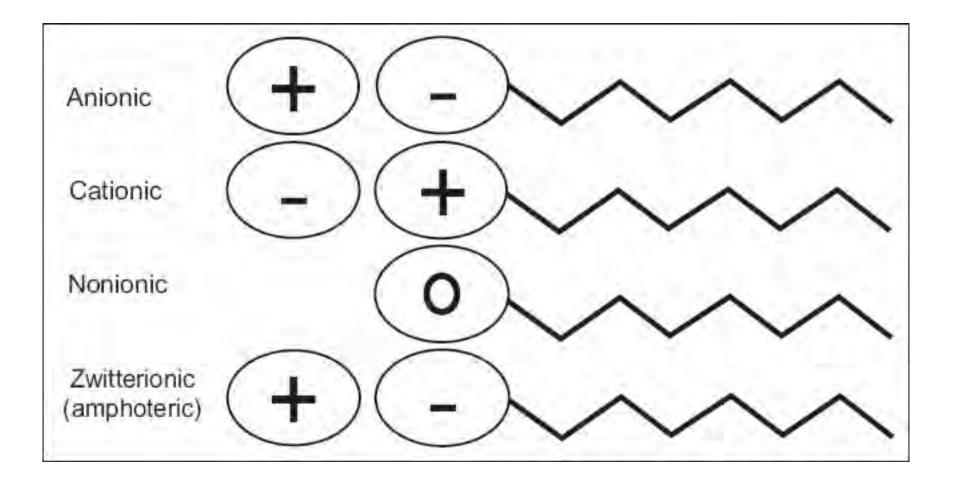
- Ingredients that make cosmetics work
- Cleansers
- Conditioners
- Film formers
- Drug actives
- Reactants
- Colorants
- Fragrances



#### Surfactants



#### **Types of Surfactants**



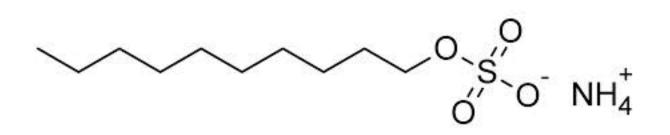
## Anionic Surfactants

- These are the primary cleansing surfactants
- Alkyl Sulfates

– Examples – SLS and ALS

Alkyl Ether Sulfates - Ethoxylated

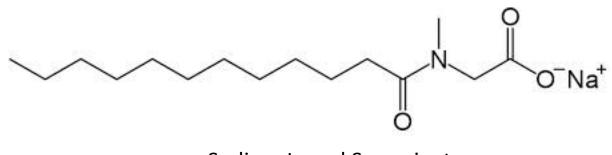
Example – SLES and ALES



## Anionic Surfactants

- Other types
  - Sulfosuccinates
  - Alkylbenzene
     Sulfonates
  - Acyl Methyltaurates
  - Acyl Sarcosinates

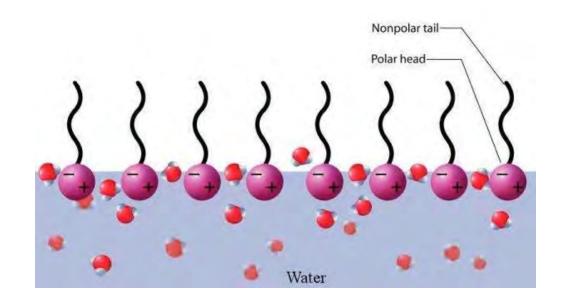
- Acyl Isethionates
- Acyl Polypeptide Condensates
- Monoglyceride Sulfates
- Fatty Glyceryl Ether
   Sulfonates



Sodium Lauryl Sarcosinate

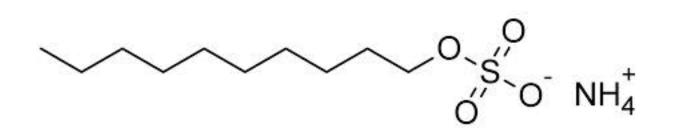
# Anionics

- Why use them?
  - Excellent detergency
  - Relatively inexpensive
  - Good foaming
  - Highly stable
- Drawbacks
  - Can be irritating
  - Drying to hair



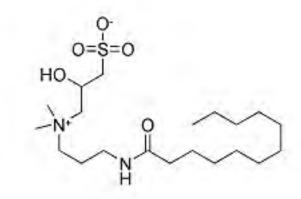
## Sulfates and Naturals

- Unacceptable for cleansing surfactants for natural products
  - Sulfosuccinates
  - Sulfonates
  - Alkyl sulfates



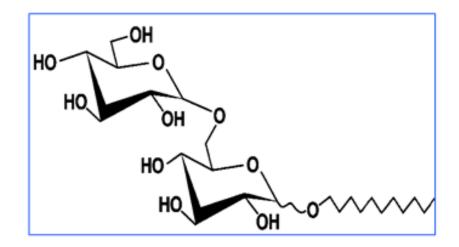
## What is used instead

- Sultaines
  - Mild secondary surfactant, more stable and better viscosity builder
    - e.g. Cocamidopropyl Hydroxysultaine
- Acyl Sarcosinates
  - High foaming secondary surfactant
    - e.g. Sodium Lauryl Sarcosinate



## Natural Surfactant Options

- Alkyl Polyglucoside
  - Natural primary surfactant derived from coconut and sugar
  - Does not build viscosity as well
  - Does not foam as well
  - Higher cost
  - e.g. Lauryl Glucoside

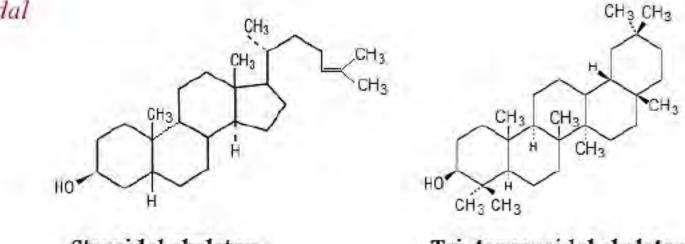


# **Saponin Glycosides**

Parts of plants containing saponins are used as detergents. For example; Root of Saponaria officinalis

#### Types:

Aglycone may be of two types; Steroidal Tri terpenoidal

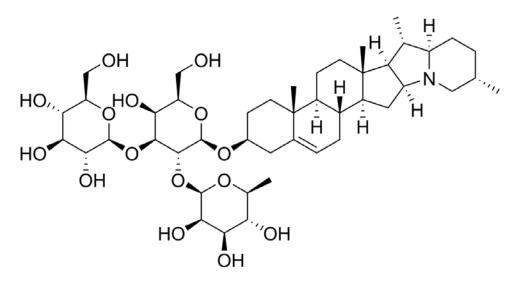


Steroidal skeleton

Tri-terpenoidal skeleton

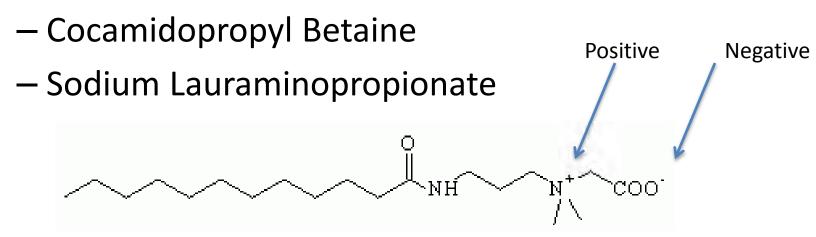
# Natural Cleansing Surfactants

- Saponins Cleansing Surfactants
- Source: plants marine derived
  - Quillaja saponaria Molina
- Difficult to purify
- Too expensive
- Not as effective
- ~40% less foam
- Highly colored



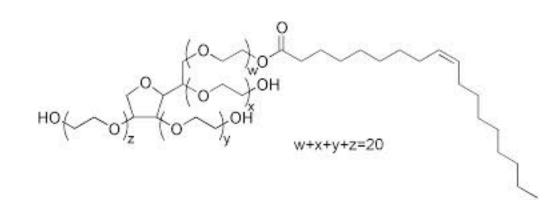
### **Amphoteric Surfactants**

- Can have a positive or negative charge depending on the pH of the solution
  - Zwitterionic
- Types



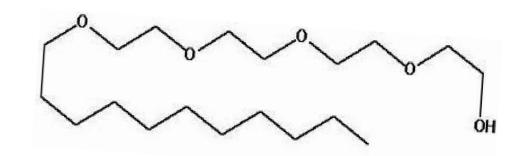
## Non Ionic Surfactants

- Surfactant molecules with no charge
- Types
  - Fatty Alcohol
  - Fatty amines
    - Lauramide DEA
  - Amine Oxides
    - Lauramine Oxide
  - Polysorbates



# Non Ionic Surfactants

- Why use them?
  - Foam enhancer
  - Reduce irritation
  - Conditioning effect
  - Solubilize fragrances
  - Emulsifiers



- Gentle Cleansers
  - PEG-80 Sorbitan Laurate
- Drawbacks
  - More expensive
  - Do not foam well on their own

#### Functional Raw Materials Conditioners & Moisturizers



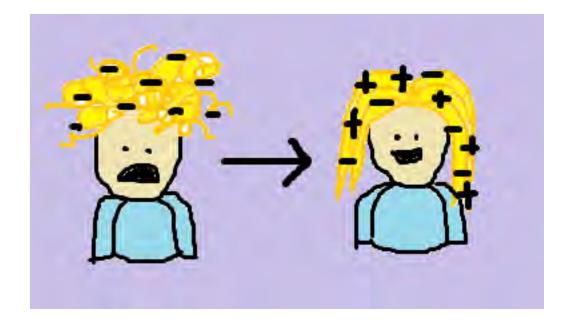
# **Moisturizing Ingredients**

- Quats
- Cationic Polymers
- Silicones
- Occlusives
- Humectants
- Emollients



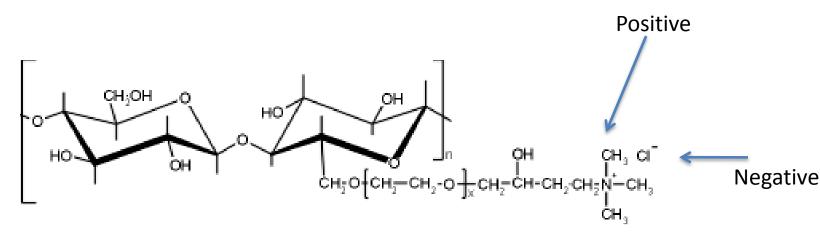
### Quats

- How do they work?
  - Electrostatic Attraction
  - More damage = more substantivity
  - Longer chain length = more conditioning



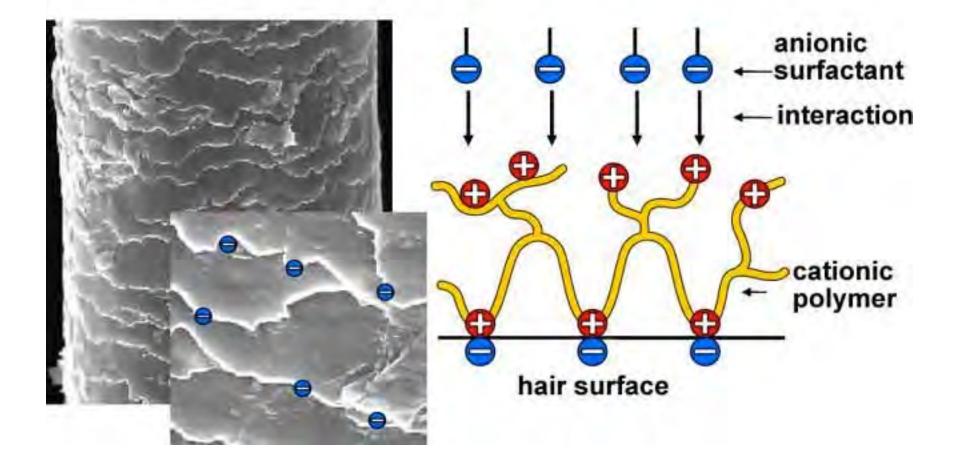
## **Cationic Polymers**

- Common Examples
  - Polyquaternium 4
  - Polyquaternium 7
  - Polyquaternium 10
  - Guar Hydroxypropyltrimonium Chloride



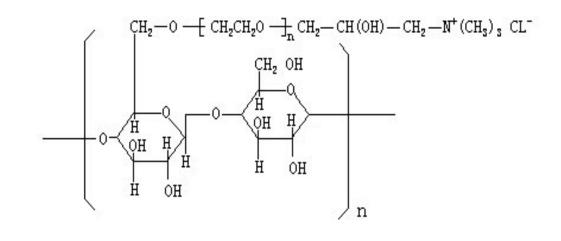
#### **Cationic Polymers**

#### Figure 1: Hair structure with cuticula Polymer - Distribution of charge



## **Cationic Polymers**

- Benefits
  - Effective at low levels
  - Compatible with anionics
- Drawbacks
   Can build-up
- % Used if formula
   Up to 5%
  - Usually 1% or less



# Silicones

- Benefits
  - Increased shine
  - Increased lubricity
  - Works on undamaged hair
  - Synergistic with cationics
- Drawbacks
  - Build-up
  - Weigh down hair
- % Used if formula
   Up to 2%

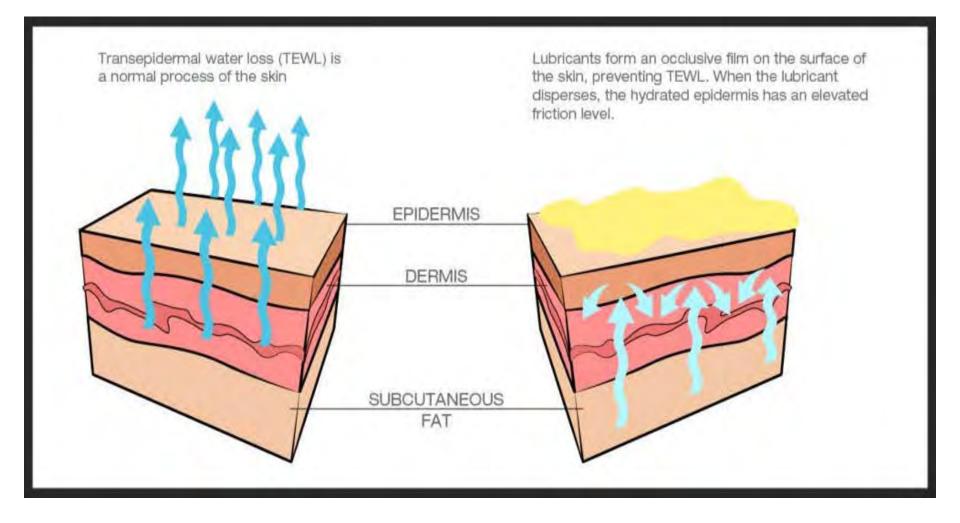


#### Humectants

- Ingredients that attract water
- Usually water soluble
  - Glycerin
  - Propylene Glycol
  - Sorbitol
  - Types of proteins
- Use level
  - 0.5% 15.0%

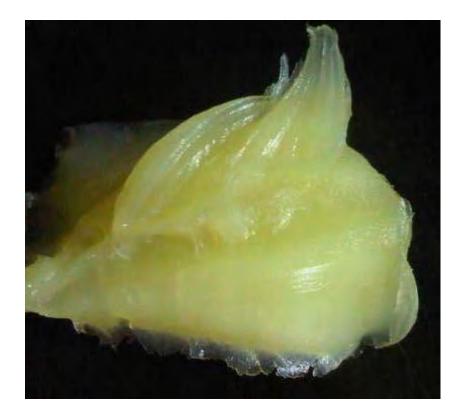
CH<sub>2</sub>OH CHOH CH<sub>2</sub>OH

### How Occlusives Work

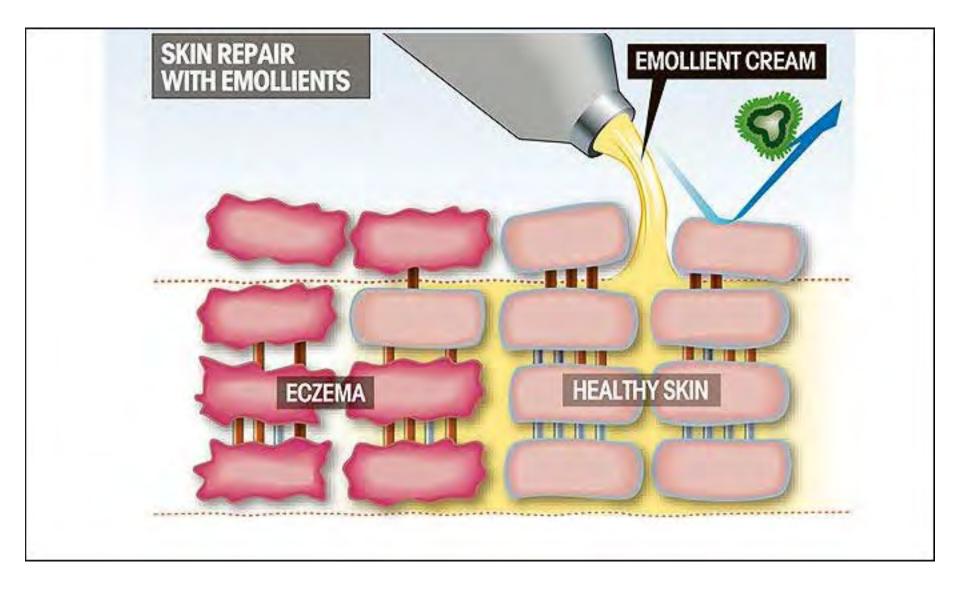


# **Occlusive Agents**

- Water-insoluble materials
- Examples
  - Petrolatum
  - Mineral Oil
  - Dimethicone
- Use Level
  - 5% to 70%



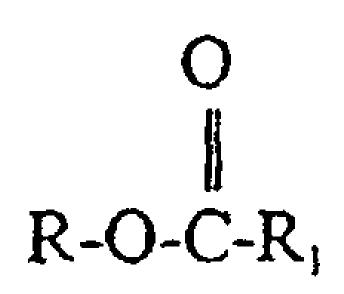
#### Emollients



# Emollients

- Light coating on skin
- Used to improve feel
- Examples
  - Coconut oils
  - Almond oil
  - Esters
  - Silicones
- Use level

- 5% - 25%



Functional Raw Materials Active Ingredients

- Proven to have an effect on cells or fight disease
- Classified as OTC Drugs
  - FDA Monograph
  - In US & elsewhere



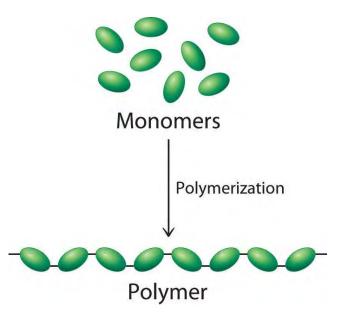
# OTC "cosmetic" Active Ingredients

- Sunscreens
- Anti-acne
- Anti-perspirants
- Anti-dandruff
- Anti-cavity
- Anti-fungal
- Anti-microbial
- Hair growth
- Skin bleaching
- Wart Remover



#### Functional Raw Materials Film Forming Polymers

- Polymers Long chain molecules made up of repeating unit molecules (monomers)
- Wide range of uses
  - Thickeners
  - Conditioning / moisturizers
  - Hair colors
  - Styling polymers



# Functional Raw Materials Reactive Ingredients

- Ingredients that chemically react to produce an effect
- Hair colorants
- Relaxers
- Perms
- Sunless Tanners
- Depilatories



# **Cosmetic Chemistry Quiz**

Which ingredient is NOT something you could possibly find in a cosmetic?

•Whale Vomit

Sheep placenta

Cow bone marrow

•Bull Semen

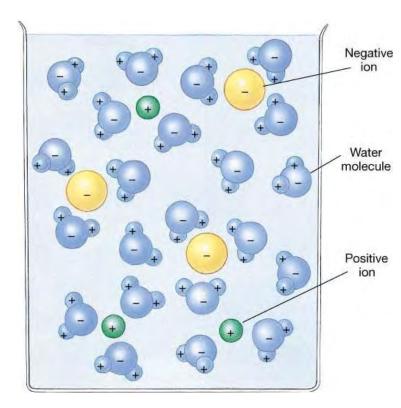
## Aesthetic Raw Materials

- Solvents
- Emulsifiers
- Adjusters
- Preservatives
- Thickeners
- Fragrance
- Fillers
- Delivery Systems



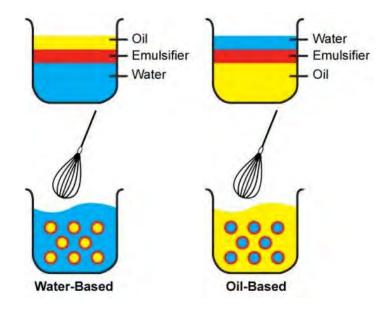
# Solvents

- Ingredients that dilute functional ingredients
- Aid in delivery
- Low cost
- Non-reactive / Compatible
- Most common
  - Water
  - Alcohol
  - Mineral Oil
  - Propylene Glycol



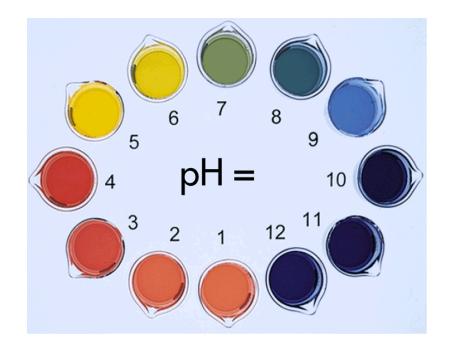
# Emulsifiers

- Ingredients that create oil & water mixtures
- Basis for all creams & lotions
- Emulsions consist of
  - Internal phase
  - External phase
  - Emulsifier
- Very few natural emulsifiers



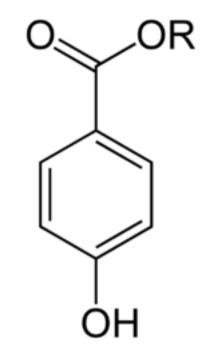
# **Formulation Aids**

- Ingredients that adjust formulation properties
  - pH
  - Viscosity
  - Solubilizers
- Acids, bases or salts
- Chelating agents
- Nonionic surfactants



## **Cosmetic Preservatives**

- Parabens
  - Propylparaben
  - Ethylparaben
  - Methylparaben
- Formaldehyde donors
- Phenol derivatives
  - Phenoxyethanol
- Quats
- Alcohol
- Organic compounds
  - Methylchloroisothiazolinone



#### Aesthetic Raw Materials

Thickeners – Ingredients that increase the thickness of a formula



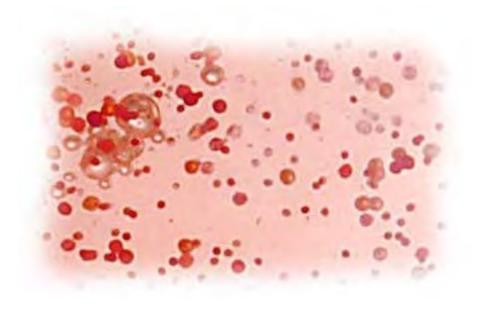
# Lipid Thickeners

- Composed of lipophilic materials
- Solid at room temperature
- Liquid when heated, solid when cooled
- Examples
  - Carnauba wax
  - Cetyl Alcohol
  - Stearyl Alcohol



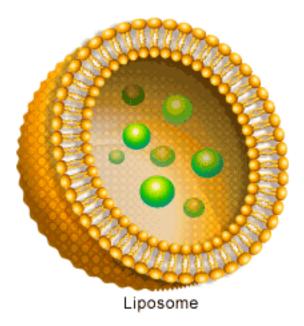
## **Appearance Modifiers**

- Pearling Agents Opacify formula
- Suspended beads
- Texture modifiers



# **Delivery Systems**

- Ingredients used to better deliver functional ingredients to skin & hair
- Cyclodextrins
- Matrix Polymers
- Liposomes



# Marketing Raw Materials

- Vitamins
- Botanical Extracts
- Proteins
- Anti-Aging
- Used at low levels
- Minimal impact on performance



## Natural Raw Materials

- Depends on Standards
- Don't expect them to work as well
- They will cost more
- Consumers want products that work



# Solutions

Simplest formulation Mixture of compounds

#### Examples

- Shampoo
- Skin oils
- Aftershave



# Natural - Shampoo

	Formula Name			Batch size
	Tier 3 Natural Standard Shampoo			500
Ĺ	Purpose	INGREDIENT	%	Amt. In Batch
1	Aesthetic – Solvent	Water	42.40	212.00
2	Functional – Conditioning	Guar Hydroxypropyltrimonium Cl	0.300	1.50
3	Aesthetic – pH adjustment	Citric Acid	0.30	1.50
4	Functional – Secondary Surfactant	Cocamidopropyl Betaine	8.00	40.00
5	Functional – Surfactant	Coco Glucoside	15.00	75.00
6	Functional – Surfactant	Decyl Glucoside	20.00	100.00
7	Functional – Conditioning	Glycerin	5.00	25.00
8	Aesthetic – Thickener	Polyacrylate 33	5.00	25.00
9	Aesthetic – Opacifier	Glycol Distearate	1.00	5.00
10	Aesthetic – Fragrance	Lavender Oil	0.50	2.50
11	Aesthetic – Preservative	Caprylhydoxamic Acid & Glyceryl Caprylate & Methylpropanediol	1.00	5.00
12	Aesthetic – Thickening	Sodium Chloride	1.50	7.50
		TOTAL	100.000	500.00
	Procedure:		Specifications	
	1. Begin mixing item #1 in container. Begin heating to 70C		- 11-	
	<ol> <li>Add items #2 - #7</li> <li>At 70C add item #9. Mix for 10 min &amp; cool</li> </ol>		pH = 5.0 - 5.5 Viscosity = 4000 - 7000	
	4. At 40C add items #10, 11 and 12		viscosity =	1000 - 1000
	5. At <30C mix 10 - 15 min			
	6. Check pH and viscosity. Adjust as requi	red		

# Emulsions

Mix of Oil & Water Held together with Emulsifier

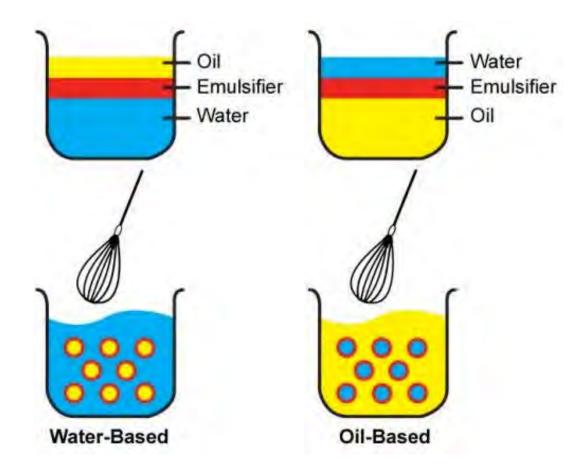
Examples

- Lotions
- Conditioners
- Moisturizers



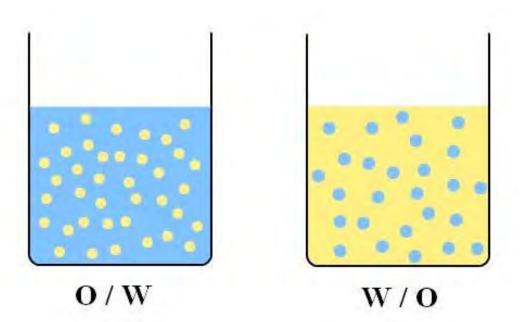
# **Emulsions Components**

- Internal phase
  - Discontinuous phase
- External phase
  - Continuous
     phase
- Emulsifier



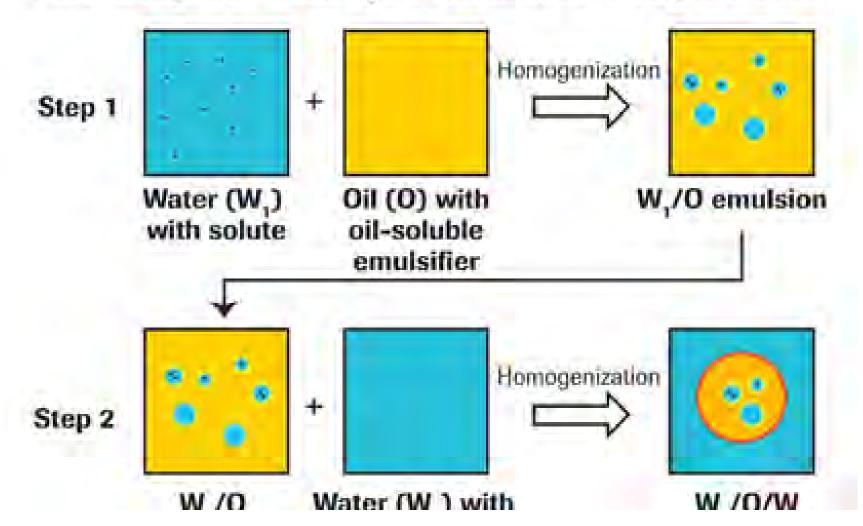
# **Emulsions Types**

- Configuration
  - Oil in Water (O/W)
  - Water in Oil (W/O)
  - Multiple emulsions (W/O/W)



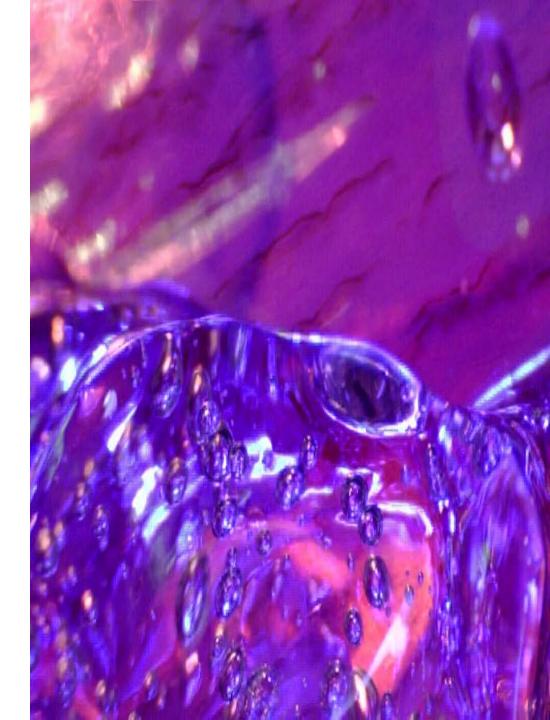
# **Multiple Emulsions**

#### **Two Steps of Multiple Emulsion Preparation**



# Gel formula

• Thickened solution or emulsion



# Types of Gel

- Styling Gels
  - Normal Hold
  - Extra Hold
- Shaving gel
- Hand gels



#### Natural Styling Gel

	Formula Name		F	Batch size
	Tier 3 Natural Standard Gel			500
-	Purpose	INGREDIENT	%	Amt. In Batch
1	Aesthetic – Solvent	Water	90.400	452.00
2	Functional – Conditioning	Sorbitol	2.500	12.50
3	Functional – Conditioning	Glycerin	3.500	17.50
4	Functional - Hold / Thickening	Dehydoxanthan Gum	2.000	10.00
5	Aesthetic – Preservative	Benzyl Alcohol	1.000	5.00
6	Aesthetic – Fragrance	Fragrance	0.200	1.00
7	Functional – Hold	Acacia Gum	0.400	2.00
		TOTAL	100.000	500.00
	Procedure:		Specifications	5
<ol> <li>Begin mixing item #1 in container. Begi</li> <li>Add items 2,3, &amp;4</li> <li>Premix item 5&amp;6. Add to formula</li> </ol>		gin heating to 45C	all al	
				pH = 5.5 - 6.0 Viscosity = 15,000 - 20,000 cp
	4. Cool to 30C. Add item #7		viscosity - i	0,000-20,000 0
	4	1		



# Cosmetic Chemistry Quiz

Which one is the FAKE beauty gadget?

- Ceramic unipolar magnet that controls acne
- Wand that shoots oxygen into your skin to smooth, tone & stimulate
- Hand held laser that makes your hair grow
- Electronic headband that relaxes muscles to remove wrinkles

#### **Creating Cosmetic Formulas**



# Sources for Starting Formulas

Patents Books Harry's Cosmeticology **Chemical suppliers** Prospector.com Trade journals Happi.com Colleagues Ingredient lists – LOIs



"Chelators work by binding trace metals like iron, which are needed for survival by microorganisms. In shampoo formulations, they can improve foam and prevent hard water bathroom deposits."

# Getting information from patents

- Google patents
- Sections of patent
- Finding formulas
- Finding testing ideas
- Working around patents

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#### **Knockout Results**

	pH	Viscosity	Foam
Control Formula	5.5	9000	8
Sodium Lauryl Sulfate	6.0	4000	3
Sodium Laurylmethosulfate	5.7	6000	4
Sodium Chloride	5.5	500	8
Cocoamide DEA	4.8	2000	5
Glycerin	5.4	9000	8
Fragrance	5.5	12000	10