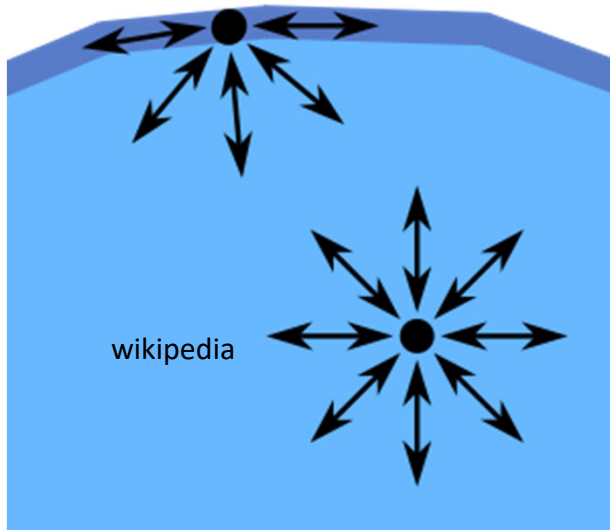


Surfactants – Soaps – Detergents



Surface tension = forces on molecules at a liquid-air interface are different from those felt by molecules in the bulk liquid

Surface tension keeps objects with higher density **'floating'**



Surfactant - micellization

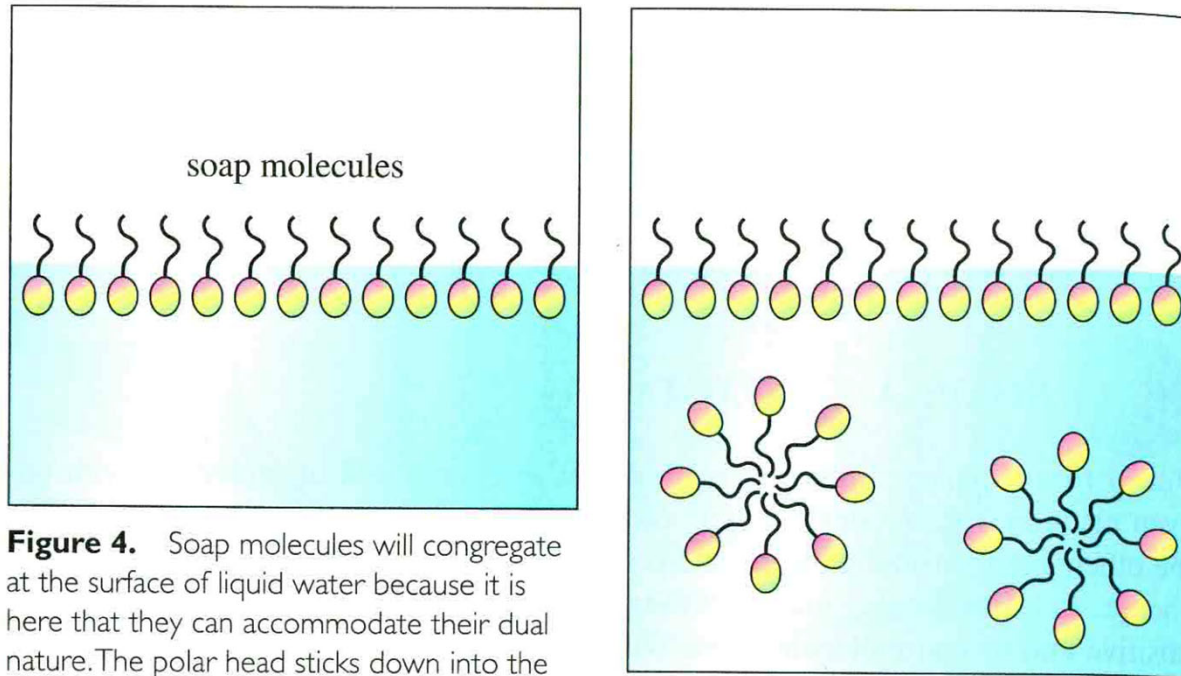
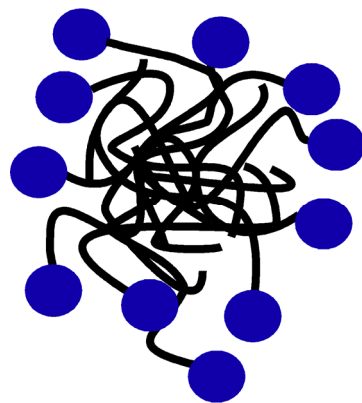


Figure 4. Soap molecules will congregate at the surface of liquid water because it is here that they can accommodate their dual nature. The polar head sticks down into the water while the nonpolar tails stick up out of



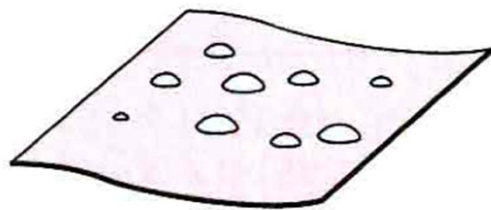
Dynamic and not symmetric

Monomer residence time - μs

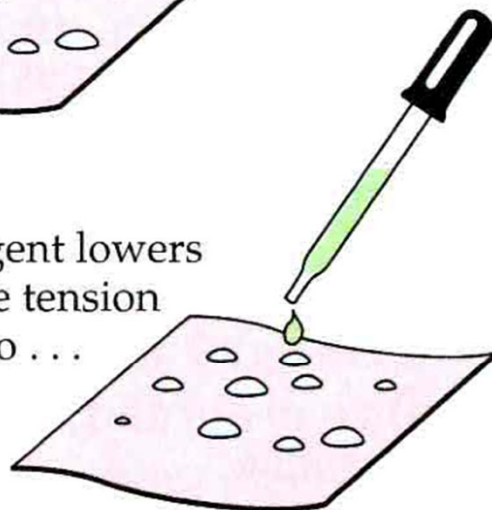
Micelle lifetime - ms

How do detergents clean?

Water's surface tension causes it to bead on the surface of fabrics.

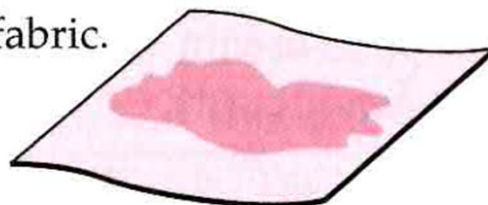


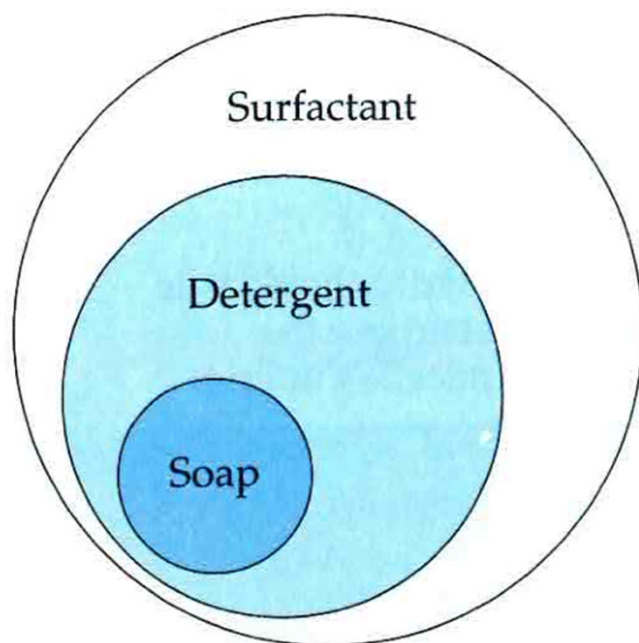
Adding detergent lowers water's surface tension and allows it to . . .



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. . . penetrate into the fabric.





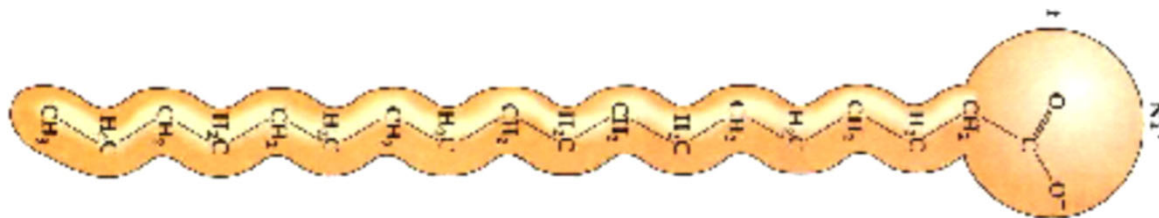
**All soaps are detergents and
all detergents are surfactants**

Soaps/detergents = hydrophobic part + hydrophilic part

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Hydrophobic = does not like water

Hydrophilic = likes water



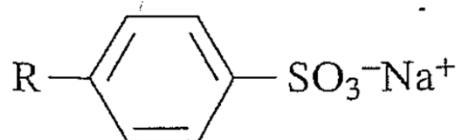
Typical detergents

Figure 13.20 Typical detergents.

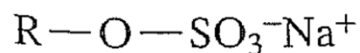
Anionic:



A sodium
alkylcarboxylate
(a soap)

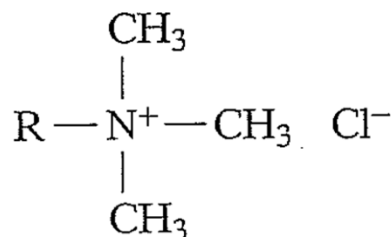


A sodium
alkylbenzenesulfonate

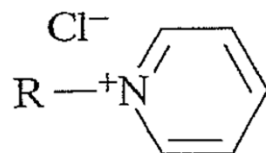


A sodium
alkylsulfate

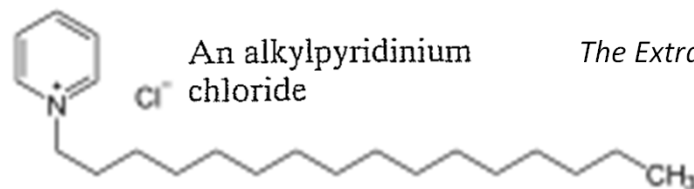
Cationic:



An alkyl
trimethylammonium
chloride

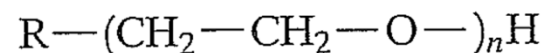


An alkylpyridinium
chloride



**Mouthwash and toothpaste
Component: antiseptic**

Nonionic:



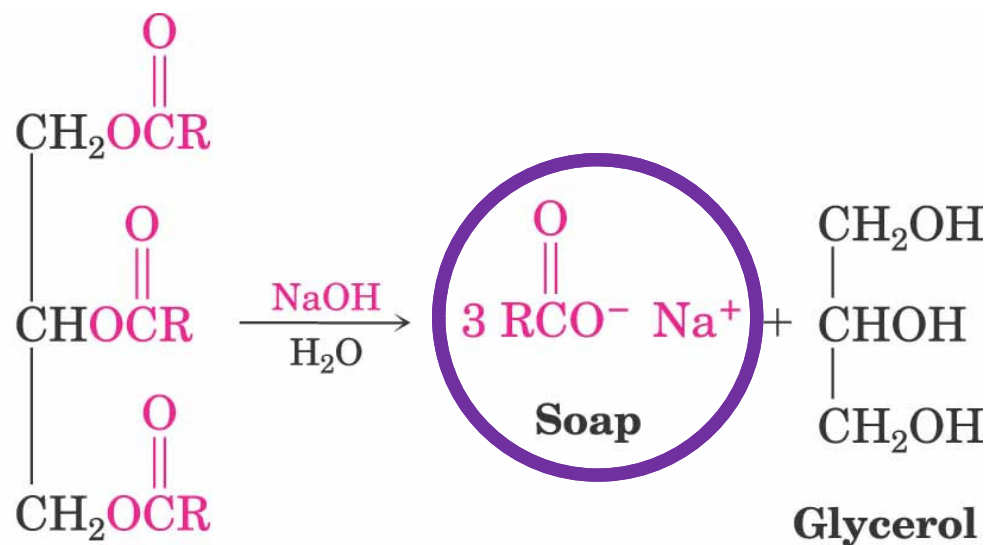
An alkyl polyethoxylate

**PEG-type long
chain alcohols**

In all these structures,
R represents a long carbon chain

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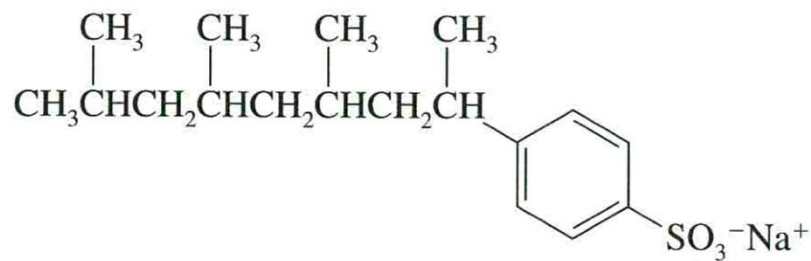
Fatty acids as soaps -saponification



A fat
(R = C₁₁–C₁₉ aliphatic chains)

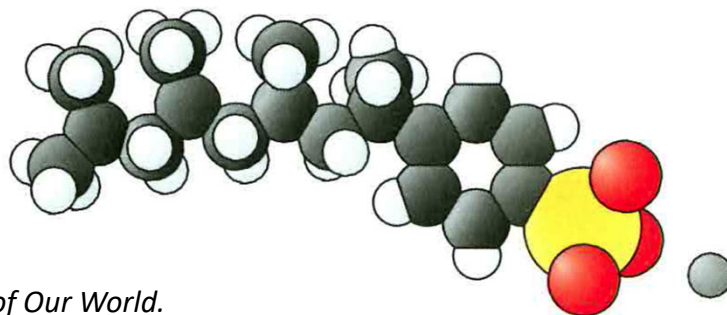
©2004 Thomson - Brooks/Cole

ABS detergent



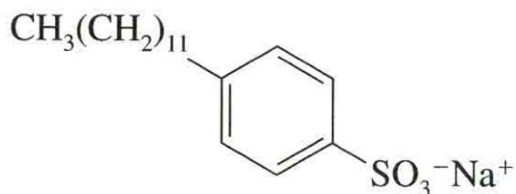
Alkyl (branched) benzene sulphonates

- Causes foaming
- Not biodegradable



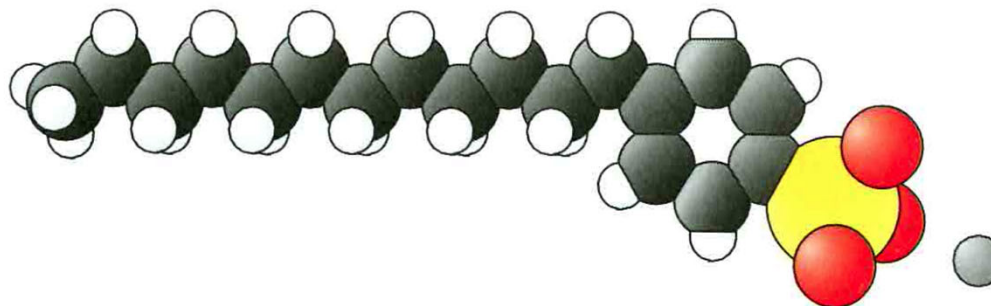
Chemistry in Focus: A Molecular View of Our World.

LAS detergent



Linear alkyl benzene sulphonates

- Non-foaming
- Biodegradable



ABS detergents are not easily degradable: build-up a problem
LAS detergents are degradable because the alkyl chain can be attacked by microorganisms

**Remarkable differences due
To small structural changes**



Table 13.4 Components of a Typical Detergent Formulation

	Component	Example	Function
active →	Surfactants	Sodium alkylbenzenesulfonates	Detergency
	Builders	Phosphates, zeolites	Soften water and increase surfactant's efficiency
helpers	Fillers	Sodium sulfate: Na_2SO_4	Add to bulk of detergent and keep detergent pouring freely
	Corrosion inhibitors	Sodium silicates: Na_2SiO_3 , $\text{Na}_2\text{Si}_2\text{O}_5$, Na_4SiO_4	Coat washer parts to inhibit rust
	Suspension agents	Carboxymethylcellulose (CMC)	Help keep dirt from redepositing on fabric
	Enzymes	—	Remove protein stains, such as grass and blood
	Bleaches	Perborates	Remove stains
	Optical whiteners	Fluorescent dyes	Add brightness to white fabrics
cosmetic	Fragrances	—	Add fragrance to both the detergent and fabrics
	Coloring agents	—	Add blueing effect

Cosmetics and Personal Care

Personal care consumer chemicals:

- hair care products
- perfumes and colognes
- skin care products and emollients (skin softening and smoothing)
- hand, face and body soaps

Cosmetic: anything intended to be applied to the human body

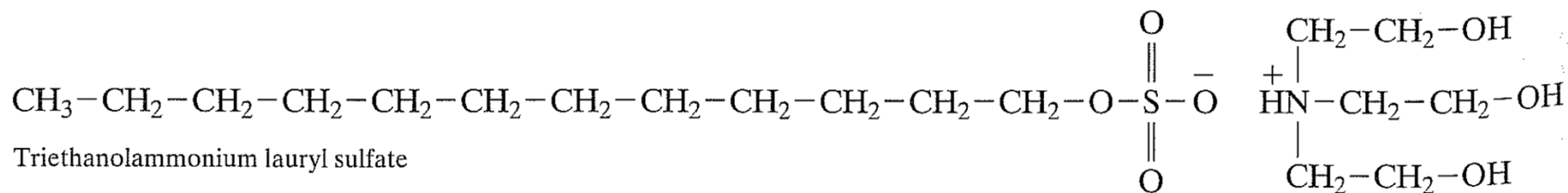
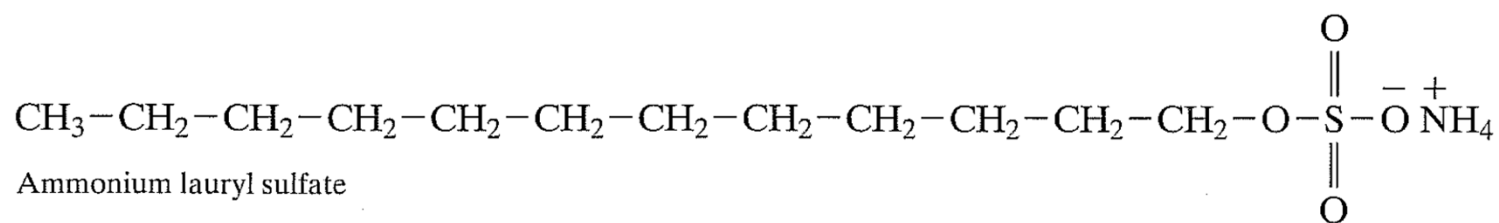
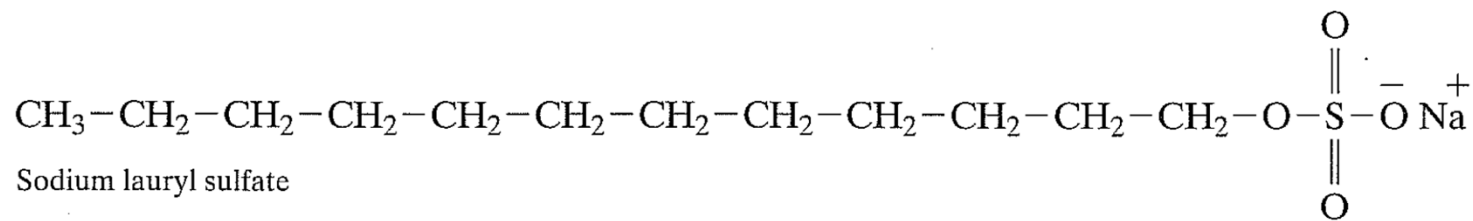
- surfactants
- fragrances

Formulations:

- primary function, e.g. cleaning
- secondary function, e.g. fresh tasting tooth paste
- convenient to use and appearance linked to intended function

Personal Care Surfactants

Figure 22.2 Surfactants of toothpastes and shampoos.



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Toothpaste



abrasives
detergents
flavorings
protective ingredients

Enamel made out of hydroxyapatite = $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$

Typical abrasives

Abrasive	Formula
Calcium carbonate	CaCO_3
Calcium pyrophosphate	$\text{Ca}_2\text{P}_2\text{O}_7$
Dibasic calcium phosphate	CaHPO_4
Hydrated aluminum oxide	$\text{Al}(\text{OH})_3$
Magnesium carbonate	MgCO_3
Talc	$\text{Mg}_3(\text{Si}_2\text{O}_5)_2(\text{OH})_2$
Titanium dioxide	TiO_2
Tricalcium phosphate	$\text{Ca}_3(\text{PO}_4)_2$

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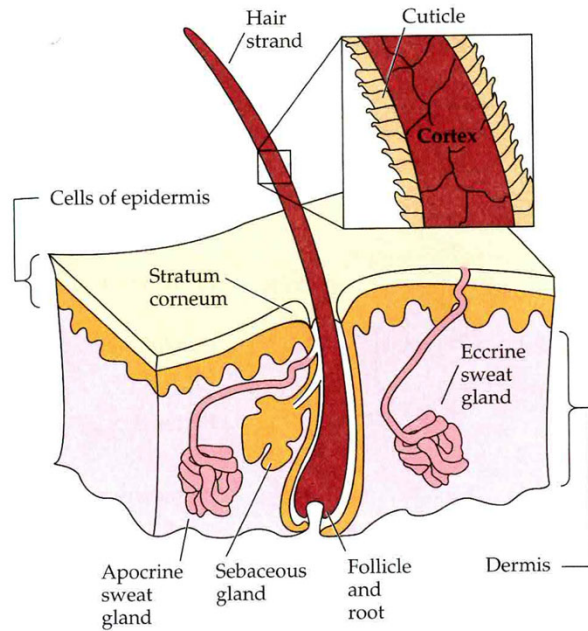
Composition of a typical toothpaste

Ingredient	Formula	Weight (%)	Function
Water	H ₂ O	39	Solvent and filler
Glycerol	$\begin{array}{c} \text{CH}_2 - \text{CH} - \text{CH}_2 \\ \quad \quad \\ \text{OH} \quad \text{OH} \quad \text{OH} \end{array}$	32	Humectant, retains moisture
Dibasic calcium phosphate	CaHPO ₄	27	Abrasive
Carrageenan	A carbohydrate of seaweed	1	Thickening agent and stabilizer
Fluorides and other additives		1	Enamel hardener; sweeteners and preservatives

Fluoride ions = SnF₂ , Na₂PO₃F, NaF

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Skin lotions



Dermis: portion of skin containing nerves, blood vessels, sweat glands, active portion of hair follicles; supports epidermis

Epidermis: outer layer consisting of several layers that grow from the bottom up

Stratum corneum: outer most layer of keratin

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Emulsion of oil and water:



skin moisturizer:

55% mineral oil, 19% rose water, 13 % spermaceti (wax from sperm whale), 12% bees wax, 1% borax

vanishing (anti-wrinkle) cream:

70% water, 20% stearic acid, 10% glycerol

Antiperspirants and deodorants

Temperature control: cooling from evaporation of water

Eccrine glands: sweat (NaCl, KCl, lactic acid, urea and glucose)

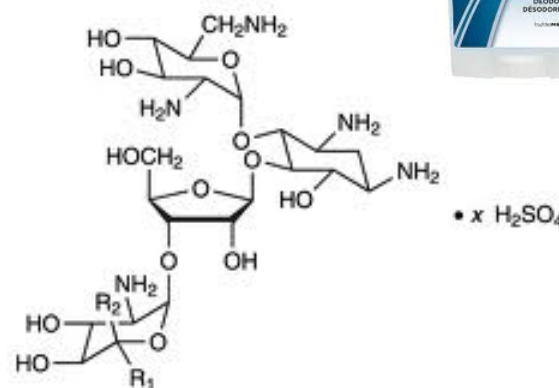
Apocrine glands: secrete fluids into hair follicles underarms, groin

- *bacteria degrade apocrine fluids = smell*

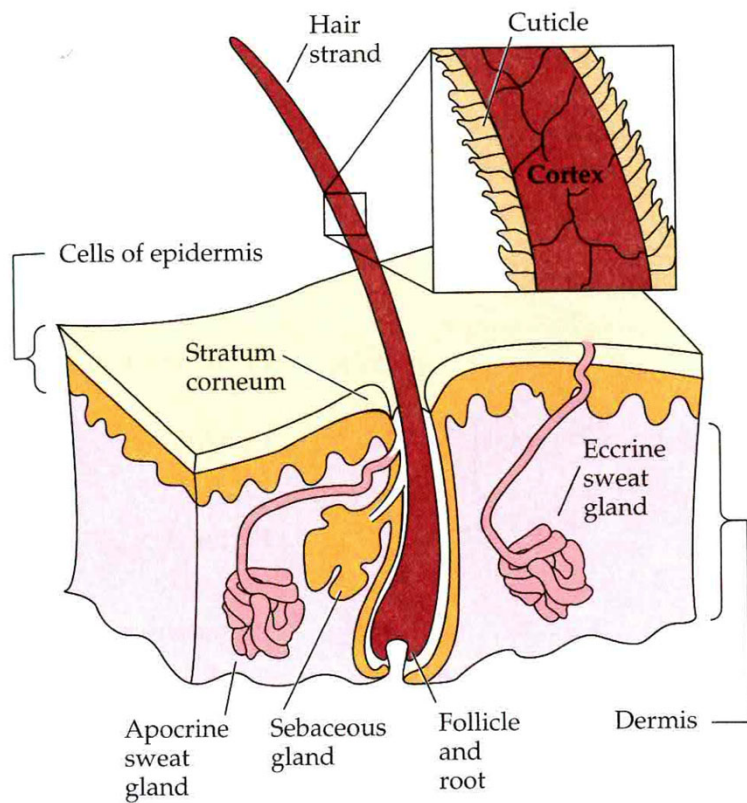
Antiperspirants: stop you sweating

aluminium chlorohydrates like $\text{Al}_2(\text{OH})_4\text{Cl}_2$ or $\text{Al}_2(\text{OH})_5\text{Cl}$

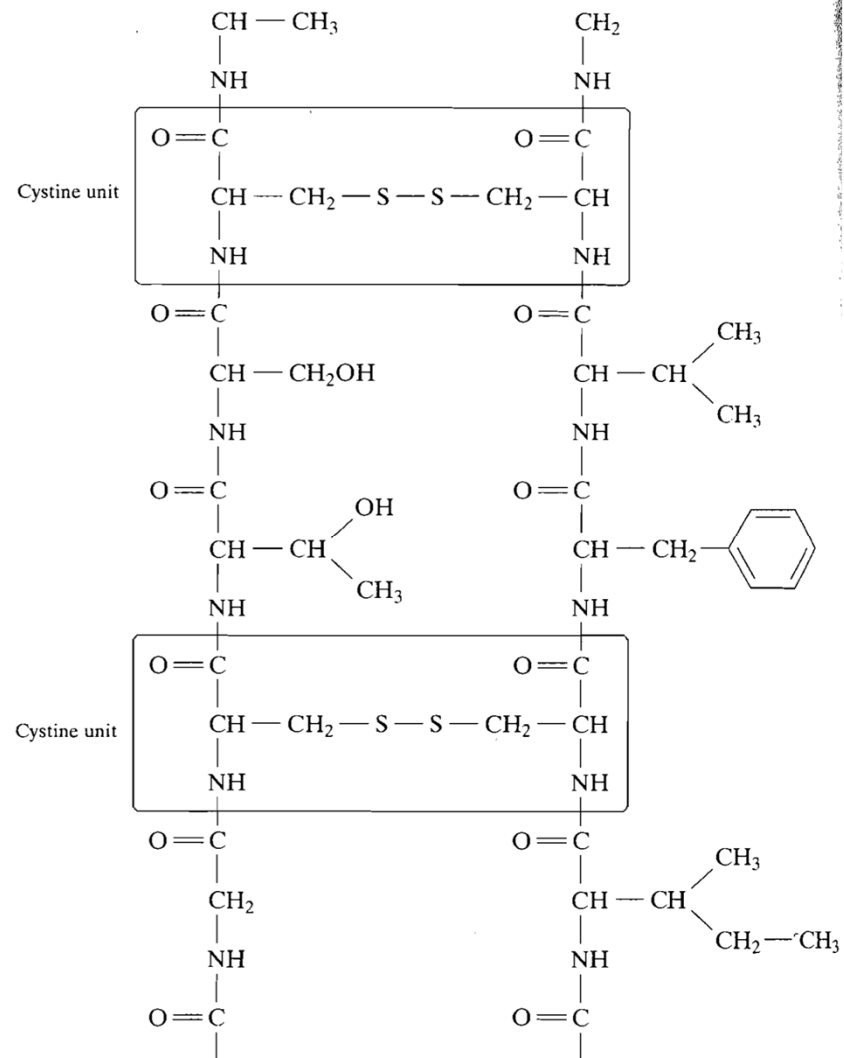
Deodorants: mask odor with fragrances
and may kill bacteria with antibiotics
(typically zinc salts of neomycin)



Hair Care Products



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Shampoo: remove dirt and excess **sebum**, but not all oil!

Conditioner replaces part of the lubricant



Table 22.1 Ingredients of a Typical Clear Liquid Shampoo

Ingredient	Weight (%)	Function
Purified water, H ₂ O	60	Solvent and filler
Triethanolammonium lauryl sulfate $(\text{HO}-\text{CH}_2-\text{CH}_2)_3\text{N}^+\text{H}^-\text{O}_3\text{SO}-\text{CH}_2-(\text{CH}_2)_{10}-\text{CH}_3$	32	Surfactant
Myristic acid, CH ₃ -(CH ₂) ₁₂ -CO ₂ H	4	pH adjustment
Oleyl alcohol, CH ₃ -(CH ₂) ₇ - $\begin{array}{c} \text{C}=\text{C} \\ \quad \\ \text{H} \quad \text{H} \end{array}$ -(CH ₂) ₇ -CH ₂ -OH	2	Conditioning agent
Fragrance	1	Perfume
Formaldehyde, $\begin{array}{c} \text{O} \\ \\ \text{H}-\text{C}-\text{H} \end{array}$	0.5	Preservative
Other additives	0.5	Sequestrants and colorants

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Acidity is important for good luster and resilience pH 4 – 6

Shampoo

Herbal Essences: pH = 5.8

Hotel shampoo: pH = 7.1

Conditioner

Neutrogena: pH 3.9

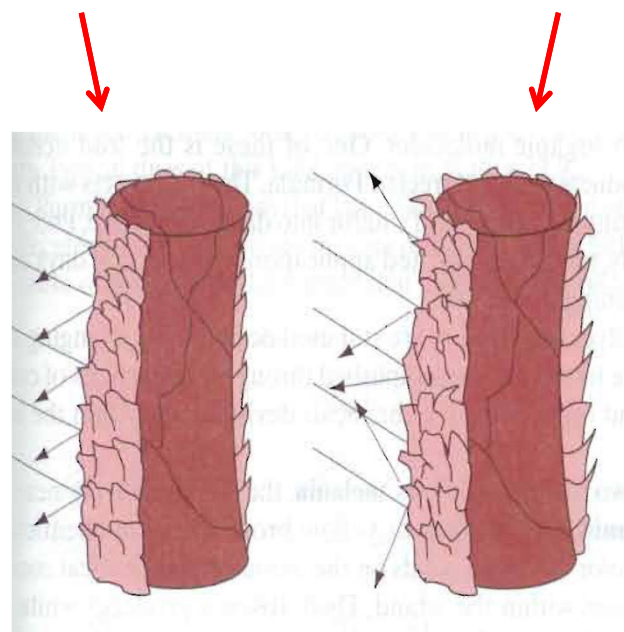
Lotion

Lorat Mayfair: pH 7.4

Measurements: A. Miller – Bohne group

OK pH

Too high a pH



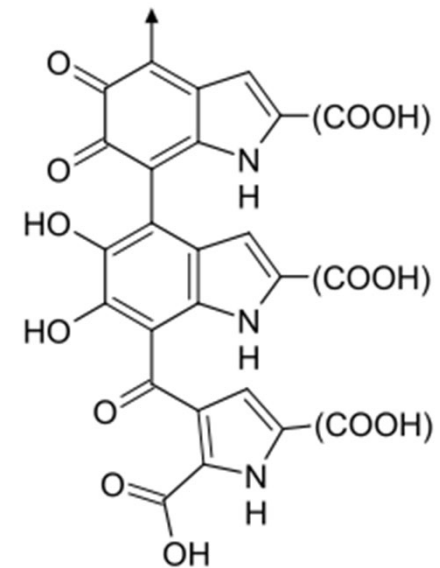
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Alignment of cuticle cells causes better reflection of light: sheen

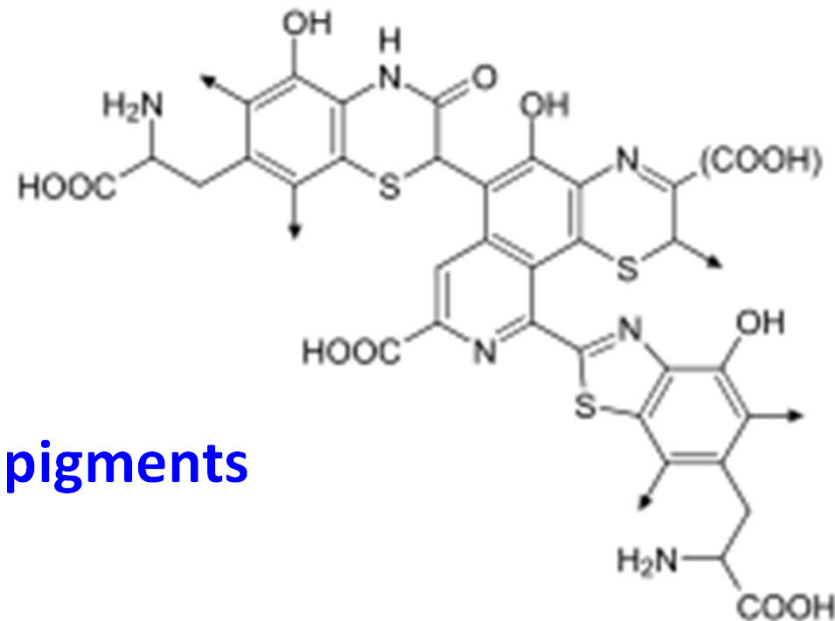
Hair colouring

Natural pigments in hair and skin

Eumelanin: black and brown variants



Pheomelanin: pink-reddish hue

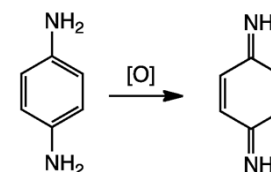
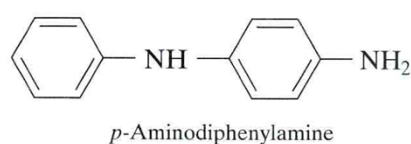
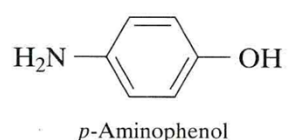
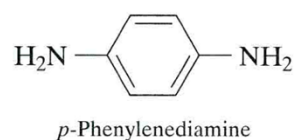


Bleaching with H_2O_2 oxidizes the pigments and they lose their colour

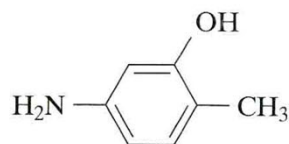
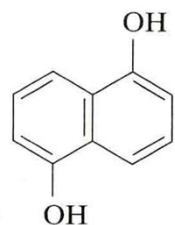
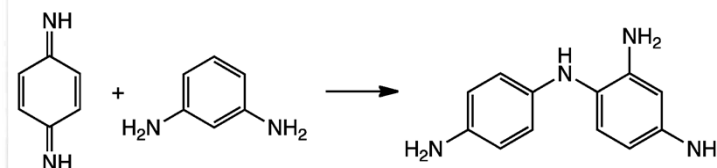
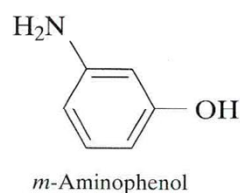
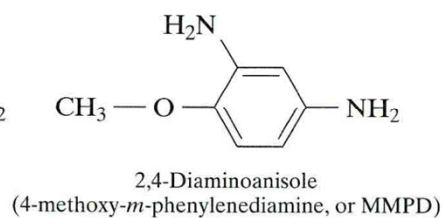
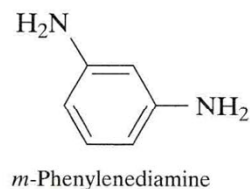
Permanent dyes

- molecules enter the cortex where the dye is formed by a chemical reaction
- H_2O_2 reacts with primary intermediate, which then reacts with the secondary intermediate to form a molecule that darkens the hair

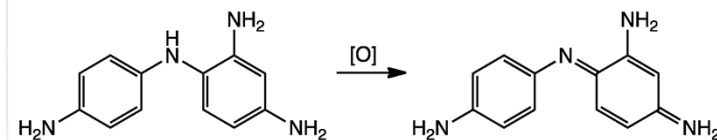
Typical primary intermediates



Typical secondary intermediates, or couplers

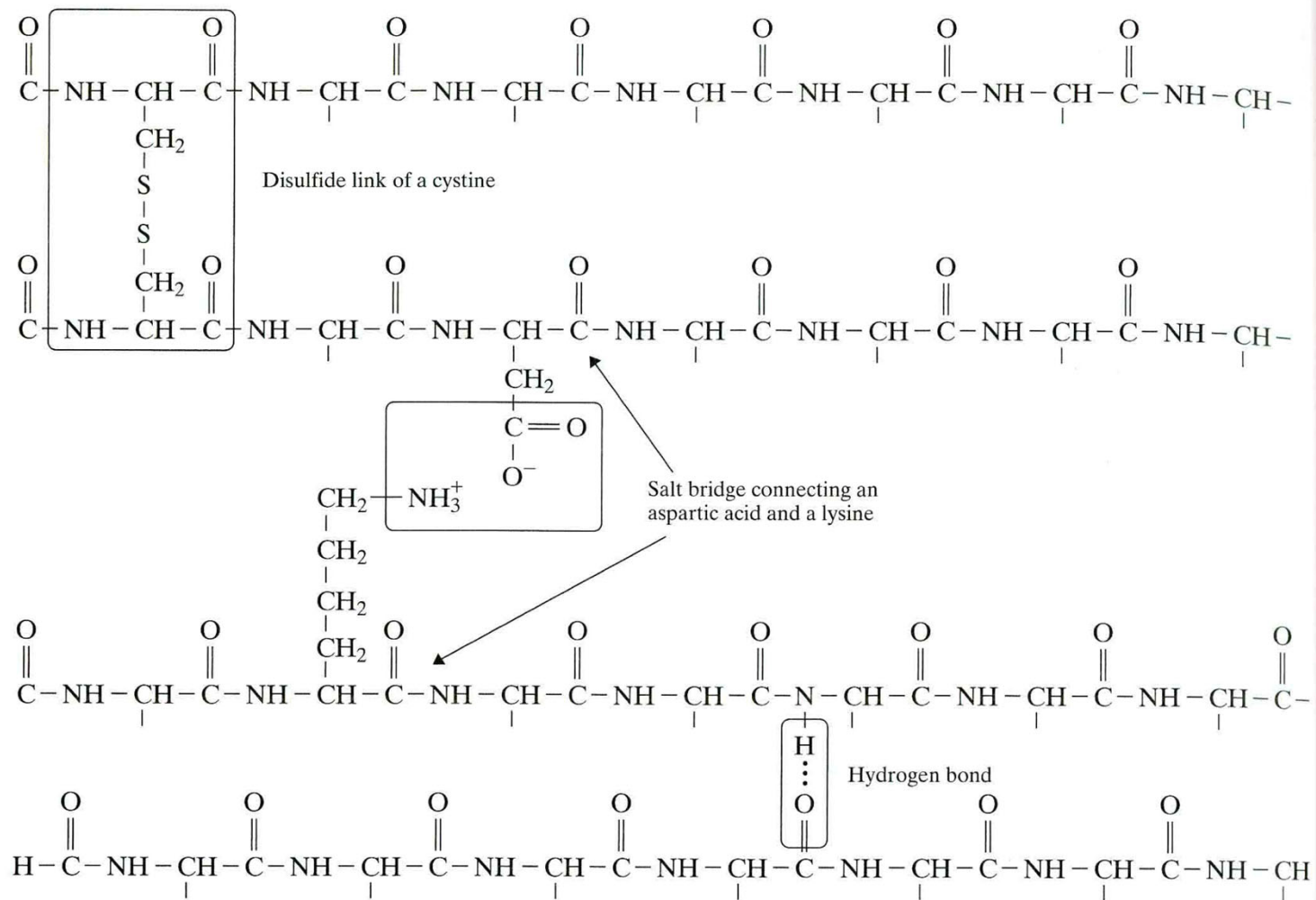


Repeat:



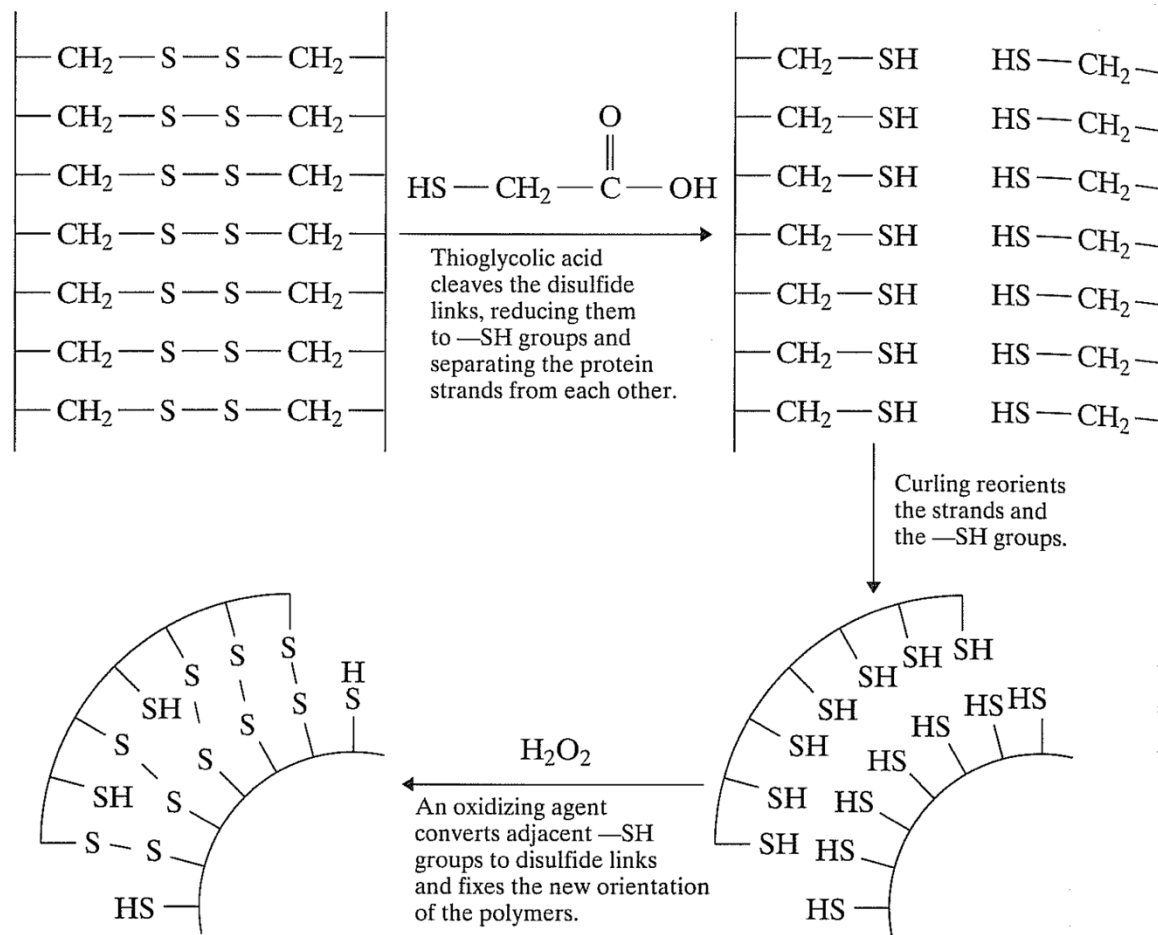
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Curling of hair



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Permanent wave: a 'perm'



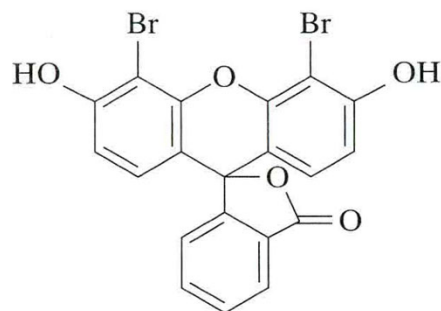
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Color on your skin

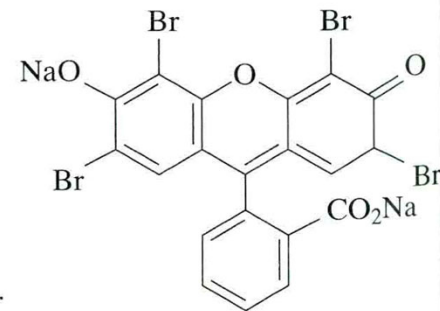
Lipstick:

- castor oil
- mixture of oils, waxes
- esters, polymers
- dyes
- perfumes
- preservatives

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D & C Orange No. 5
4',5'-dibromofluorescein



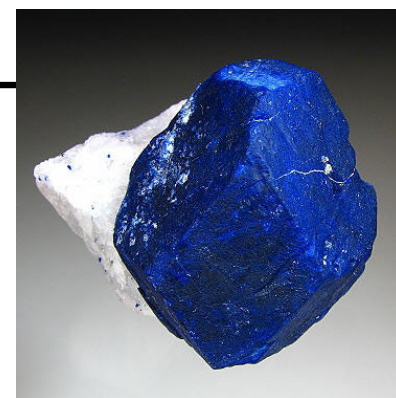
D & C Red No. 22
2',4',5',7'-tetrabromofluorescein

Mascara:

- beeswax, lanolin, hydrocarbons
- ultramarine blue – sulfur containing sodio – silicate – lazurite



- carbon black
- titanium dioxide TiO_2 – white



Face powders

Table 22.4 Composition of a Caked Face Powder

Ingredient	Weight (%)	Formula	Function
Talc	65	$\text{Mg}_3(\text{Si}_2\text{O}_5)_2(\text{OH})_2$	Forms cosmetic bulk, provides desired texture
Kaolin	10	Al_2SiO_5 , hydrated	Absorbs water
Zinc oxide	10	ZnO	Provides hiding power
Magnesium stearate	5	$\text{Mg}(\text{O}_2\text{C}-\text{C}_{16}\text{H}_{32}-\text{CH}_3)_2$	Provides texture
Zinc stearate	5	$\text{Zn}(\text{O}_2\text{C}-\text{C}_{16}\text{H}_{32}-\text{CH}_3)_2$	Provides texture
Mineral oil	2	Hydrocarbons	Emollient
Cetyl alcohol	1	$\text{CH}_3-(\text{CH}_2)_{14}-\text{CH}_2\text{OH}$	Binding agent
Lanolin and other additives	2		Softening and coloring agents, perfumes

clay



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Perfumes and Fragrances

Perfumes

- synthetic chemicals, animal oils, fragrant plant extracts
- solutions containing 10 – 25% alcohol

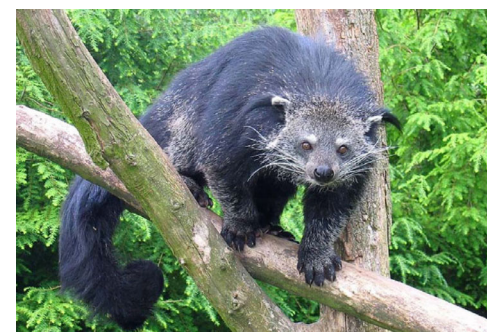


Chanel No. 5
(1920)

Cologne:

- diluted perfume (< 10% fragrances of perfume)

4000 substances from plants/animals;
2000 synthetic ones in use

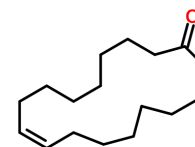


Typical perfume formulation:

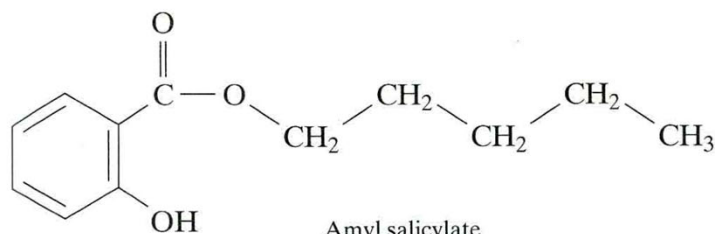
Top note – first impression: phenylacetaldehyde – hyacinths, lilacs – volatile

Middle note – stays for some time: 2-phenylethanol – roses

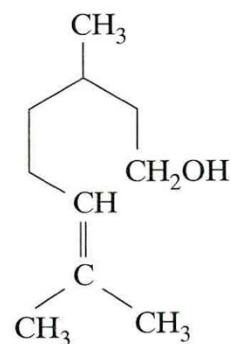
End note – residual odor: civetone – musk – civet cats



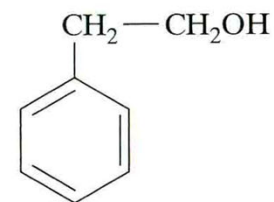
Some common fragrance chemicals:



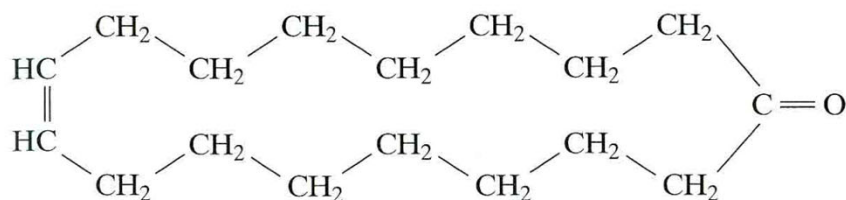
Amyl salicylate
(jasmine)



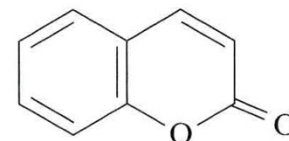
Citronellol
(roses, citrus)



2-Phenylethanol
(β -phenylethyl alcohol)
(roses)

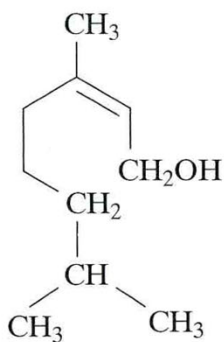


Civetone
(musk)

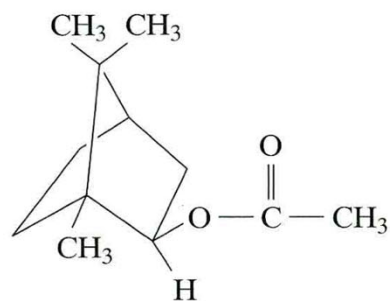


Coumarin
(sweet hay)

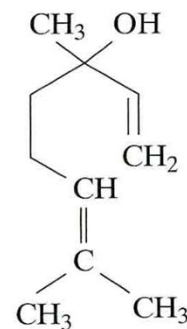
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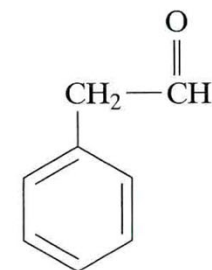
Geraniol
(roses, geraniums)



Isobornyl acetate
(pine needles)

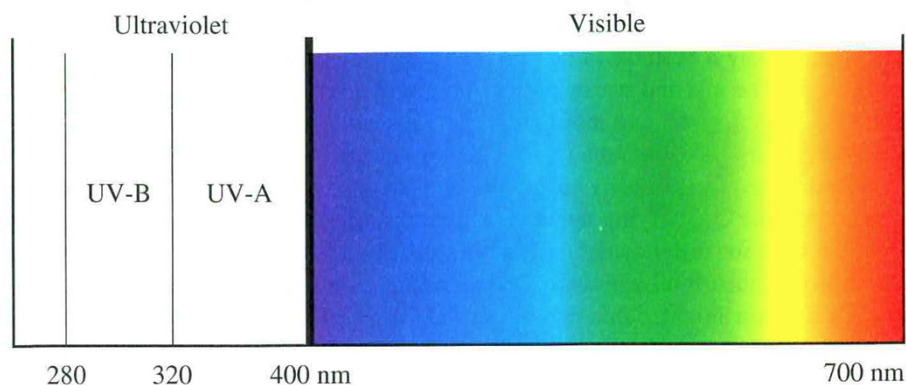


Linalool
(lavender)



Phenylacetaldehyde
(hyacinths, lilacs)

Sunscreens



UVA = 320 – 400 nm

UVB = 280 -320 nm

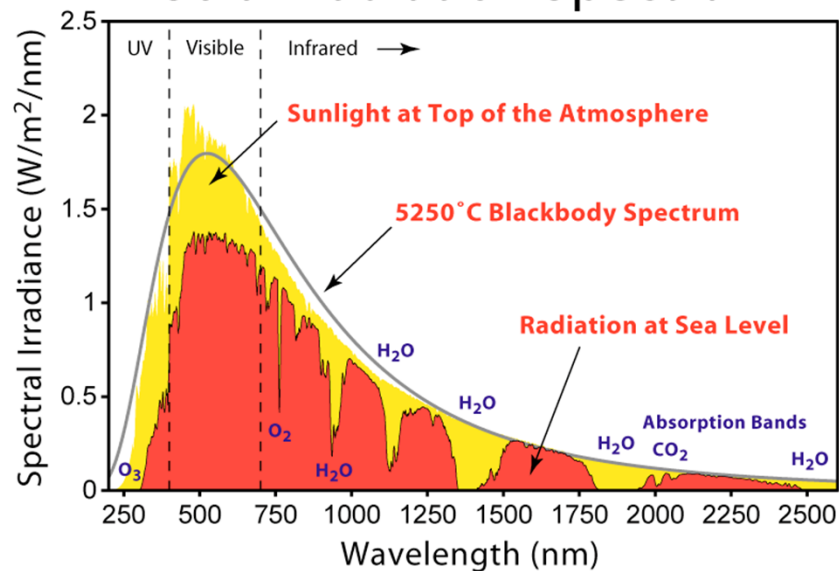
Both can cause skin cancer:
UVA penetrates deeper but UVB
deposits more energy

UVB does not pass through glass

See: <https://www.skincancer.org/prevention/uva-and-uvb>

Chemistry in Focus: A Molecular View of Our World.

Solar Radiation Spectrum

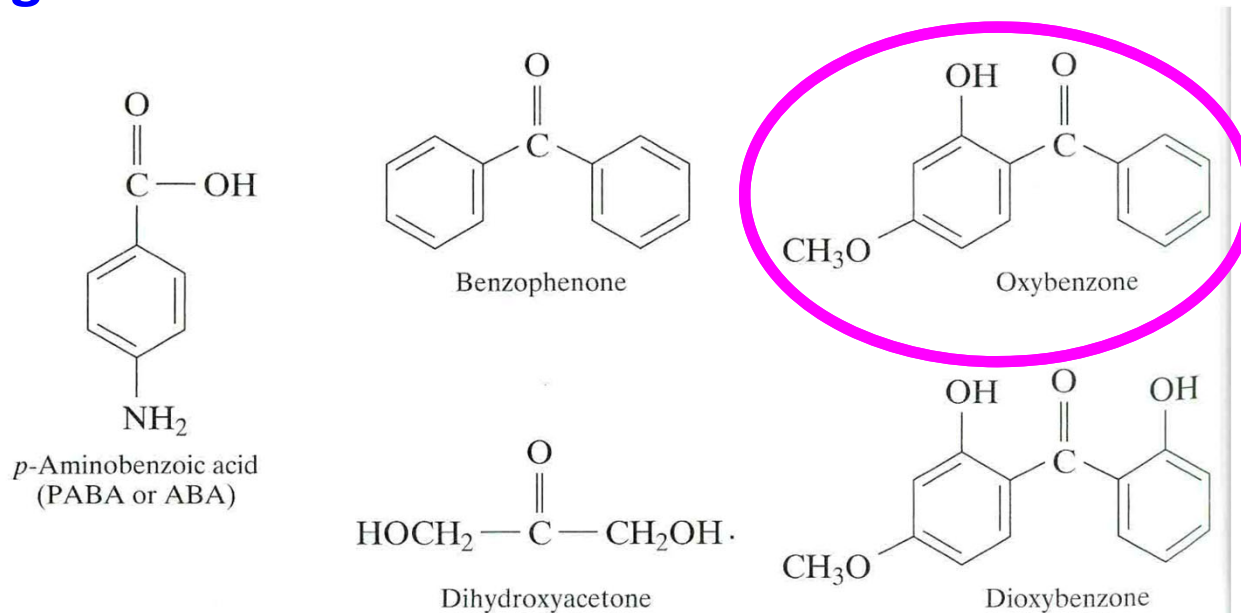


wikipedia

Two possible modes of operation:

Scatter light – opaque inorganic oxides: zinc oxide, titanium dioxide

Absorb light – small molecules:



The Extraordinary Chemistry of Ordinary Things, 4th Ed.

Oxybenzone blamed for bleaching of corral reefs and has been banned in Key West (as of Feb '19) and will be in Hawaii in 2021

<https://www.npr.org/2019/02/06/691913378/key-west-votes-to-ban-popular-sunscreen-ingredients-to-protect-coral-reef>