



## Silicones in Personal Care

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GE Silicones  
April 5, 2004



## Agenda

- Introduction to Silicones
- Sand to Specialties - Silicone Chemistry
- Silicone Nomenclature
- GE Silicones product range
- Personal care product forms
- Silicones in personal care
- Silicones in a sunscreen formulation



Atomic Symbol: Si

Atomic Number 14

Atomic Weight 28.086

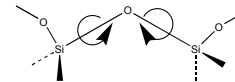
2nd Most Abundant Element

Composed of 28% of Earth's Crust

Common Form: SiO<sub>2</sub>, Sand, Quartz, Amethyst



## Structure and Characteristics



- Small Change in Physical Properties with Temperature
- Small Change in Physical Properties with Molecular Weight
- Low T<sub>g</sub> = 146 K
- Low Modulus
- High Vapor Permeability



## Silicone Physical Properties

- **Polydimethylsiloxane Backbone Flexibility**
  - Easy Orientation at Interface
  - Product Structure Diversity
- **Weak Intermolecular Forces, Free Rotation about Si-O Bond**
  - Low melting points
  - Low boiling points for lower molecular weight oligomers, Dx, MDxM, x ≤ 7
  - Small change of viscosity with temperature
  - Low Tg = 146K
  - Liquid at high molecular weights
  - Low Friction with Polymers
  - High Gas Solubility and Permeability
  - High Spreading Coefficient
- **Methyl Groups:**
  - Low Surface Tension
  - Limited Solubility in Water and Organic Solvents
  - Hydrophobic

*Silicone is Unique because of its Chemistry*

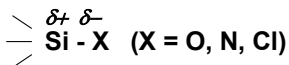


## Periodic Table of the Elements

- Should resemble Carbon Reactivity
- Actually is more like Boron
- Should be Tetra-Valent (but has empty D orbitals)
- Should be Larger than Carbon
- At border between Metals and Non-Metals



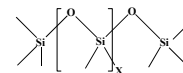
## Chemistry of Silicone Compounds Silicon vs. Carbon



- Bond is stronger than the carbon analogue
- C-O: 86 Cal/mol    Si-O: 108 Cal/Mole    C-C: 83 Cal/mol
- Silicon Radius (1.17A) is larger than Carbon (0.77 A)
- C-O: 1.43 A    Si-O: 1.6A
- Silicone is less electronegative than Carbon
  - Bonds to X are more polar
- D orbitals available



### Silicone



x = 25  
x = 7000

Fluid  
Gum

Resists:

O<sub>2</sub>  
O<sub>3</sub>  
H<sub>2</sub>O  
UV  
Heat (500 F)  
Cold (-60F)  
Electricity

Attacked by:

HF  
Strong Bases  
Strong Acids  
Solvent (Swelling)  
Fire (Somewhat)  
Some Metals

### Hydrocarbon



Paraffin wax  
High density polyethylene

Acid  
Base  
Some Solvents  
Electricity

O<sub>2</sub>  
O<sub>3</sub>  
UV  
Temperature (Properties change)  
Some Solvents  
Fire (Consumed)



Nomenclature

CH4 Methane SiH4 Silane

C-OH Alcohol Si-OH Silanol

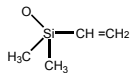
C-O-C Ether Si-O-Si Siloxane



Silanol



Alkoxy



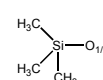
Vinyl



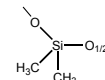
Hydride



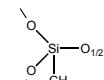
Silicone Shorthand



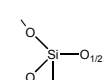
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D



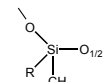
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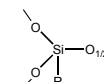
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M\*



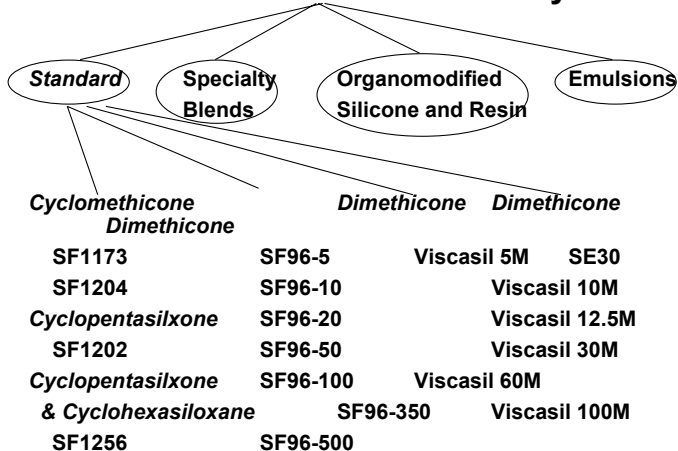
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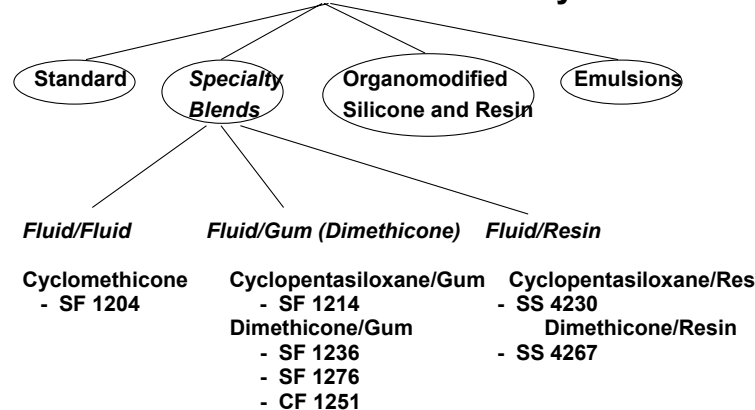
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GE Silicones PC Product Family Tree

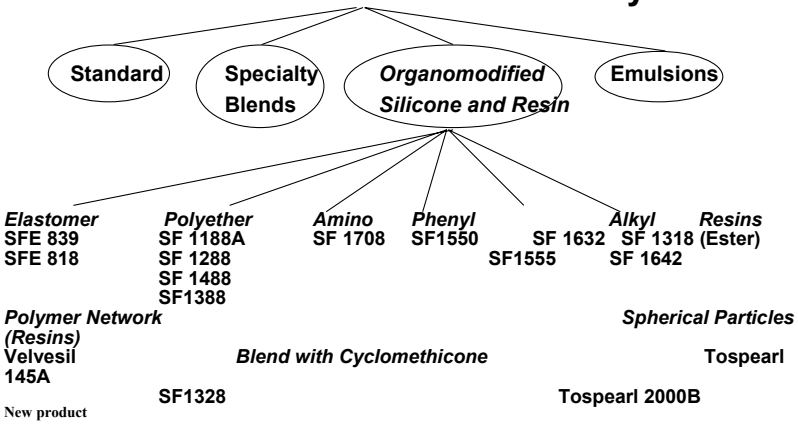


GE Silicones PC Product Family Tree

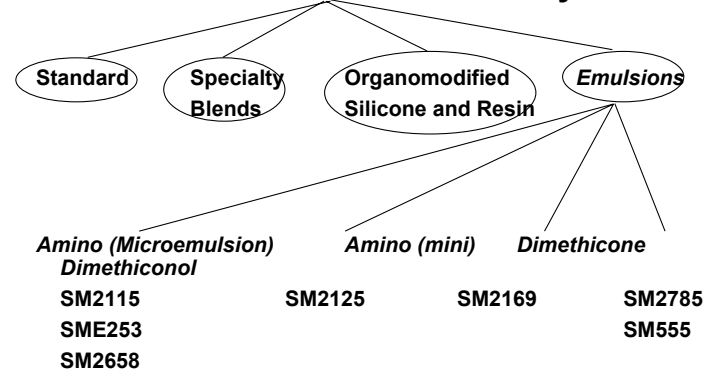




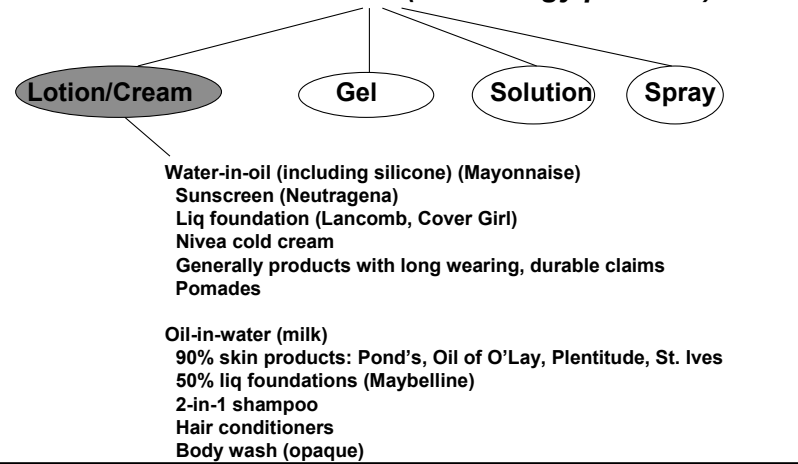
### GE Silicones PC Product Family Tree



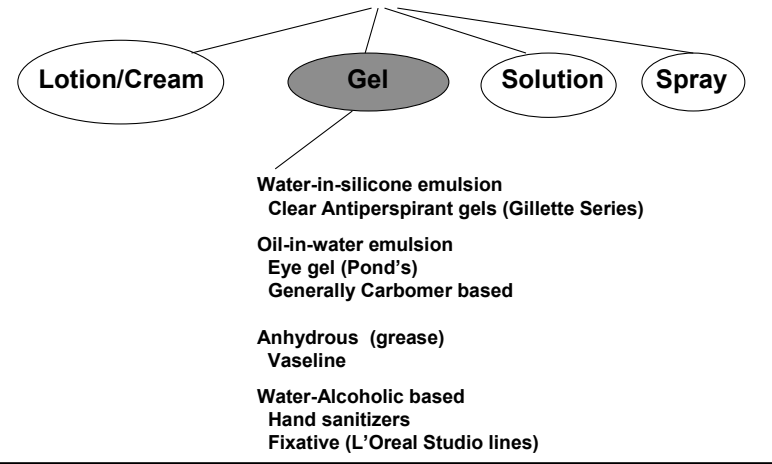
### GE Silicones PC Product Family Tree



### Product Forms (technology platform)

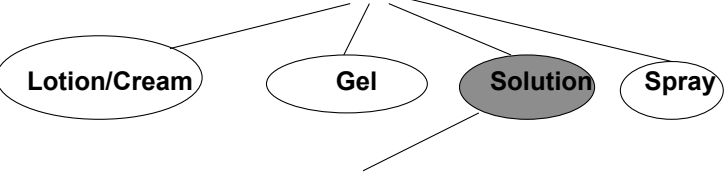


### Product Forms (technology platform)





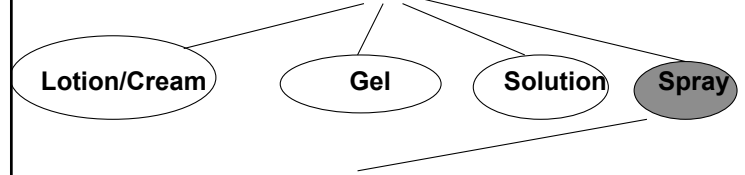
### Product Forms (technology platform)



- One phase, clear
- Dry oil spray (J & J)
- Capsules (Elizabeth Arden Green tea, Pond's)
- Serums (EA Good morning Skin Serum, Lancomb)
- Astringent
- Facial
- Clear Shampoo
- Shower gels



### Product Forms (technology platform)



- Oil-in-water emulsion
- Low viscosity (Polo Man's after shave)
- Hair detangler spray
- Solutions
- Hair spray (alcoholic/water)
- Suspension
- Antiperspirant



## GE Silicones For Personal Care

### Silicones Provide:

- The Dry Feel for Antiperspirants
- The Formulation Vehicle for Clear Gel Antiperspirants and Deodorants
- The Conditioning Agent for 2/1 Shampoos and Hair Conditioners
- A Smooth, Silky, Non-greasy Feel for Skin Care and Cosmetics
- Long Lasting Durability for Color Cosmetics
- Water Resistance for Sunscreens



## Attributes of Silicones

### Performance/Functional Benefits

- Emolliency
  - Lubricity
  - Spreadability
- Uniform film
- Fast Absorption
- Ease of Rub-in
- Play time (color)
- Delivery vehicle
- Emulsifier
- Protection (Hydrophobic)
- Cleansing (solveny, volatiles)

### Sensory Enhancement

- Soft
- Smooth Feel
- Silky Dry
- Non Greasy
- Non Oily
- Matte (skin and cosmetics)
- Shine (hair, nails, lips)
- Detackification

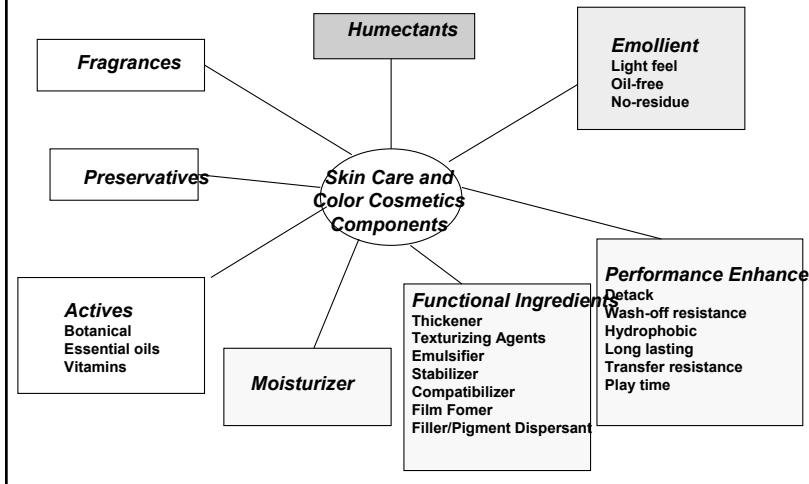
### Safety Benefits

- High Thermal and Oxidative Stability
- Non irritating
- Low Toxicity
- Non comedogenic
- Essentially Odorless

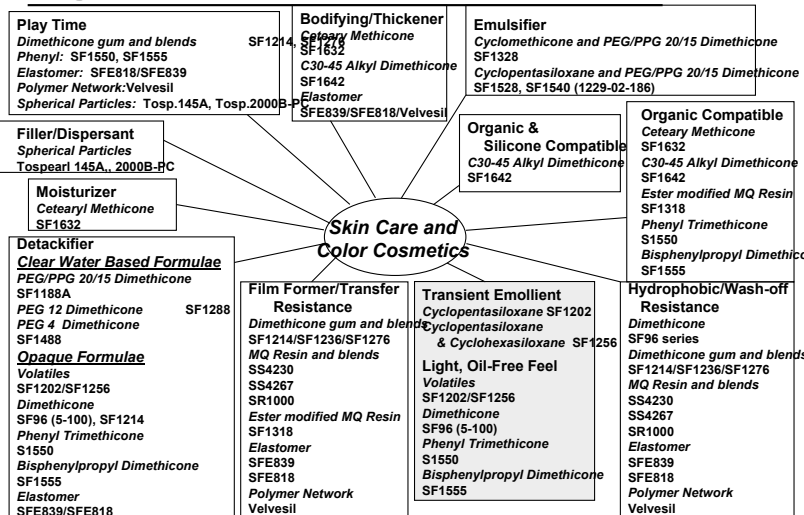


# Skin Care Components

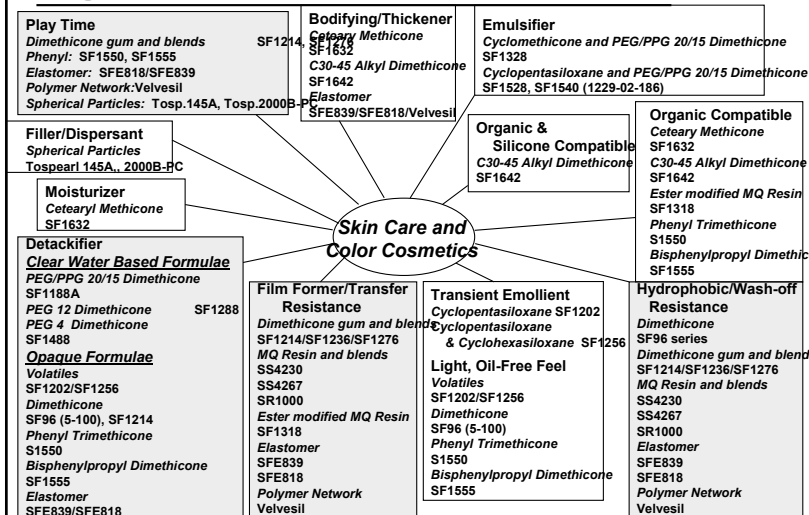
- **Emollients:** materials that make the skin feel smoother
  - Organic
  - Silicone (oil free)
- **Humectants:** materials that draw moisture to themselves
  - glycerin
  - silicones generally are not humectants (exceptions are water soluble dimethicone copolyols)
- **Moisturizers:** prevents trans-epidermal water loss (elasticity, smooth)
- **Emulsifiers:** “forces” incompatible ingredients (oil and water) together
  - Dimethicone copolyols (SF1328, SF1528) for water-in-silicone systems
- **Viscosity Control Agents:** thickeners, thinners
- **Specialty Ingredients:** Performance enhancers
  - Durable, long lasting (film formers: SS4230, SS4267)
  - Sensory enhancer, detack (SFE839, SFE818, SF1214)
- **Actives:** Vitamins, antioxidants, sunscreen actives, AHA
- **Fragrance**
- **Preservatives**



# Skin Care and Color Cosmetics

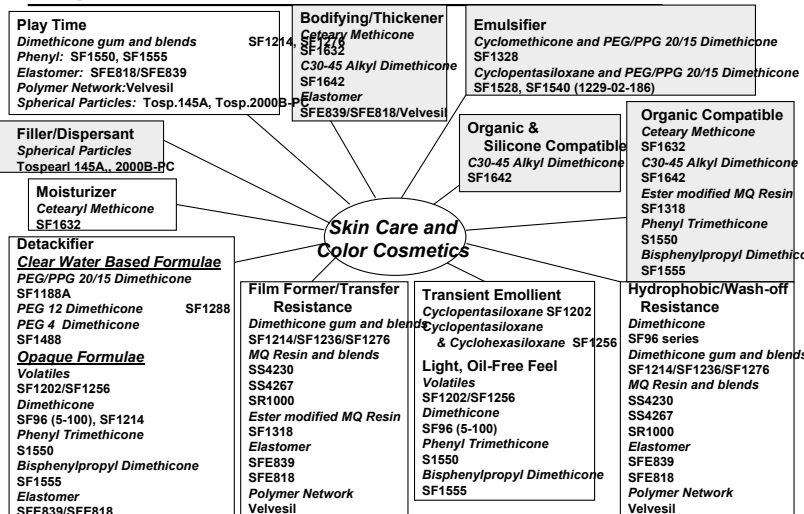


# Skin Care and Color Cosmetics

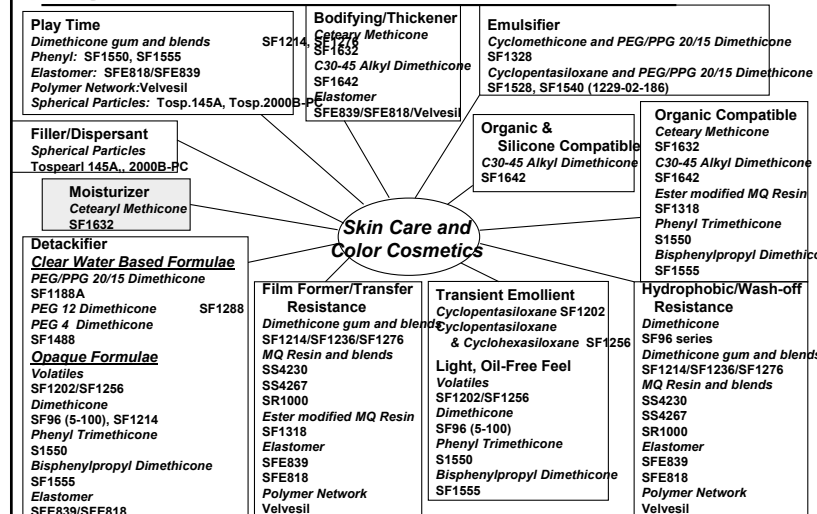




## GE Silicones



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### Silicones in Skin Care Products

<b>Cyclomethicone:</b> Transient emollient, actives carrier, detackify	1-
15%	
<b>Dimethicone:</b> Antisoaping, Antiwhitening, emollient, detackify	0.5-
5.0%	
<b>Cyclopentasiloxane &amp; Dimethicone Copolyol:</b> Emulsification vehicle	10%
<b>Gum/fluid blends:</b> Emollient, film former, water repellency, sensory	5-
10%	
<b>Trimethyl siloxysilicate:</b> Film former, durability, water-off resistance	3-
5%	
<b>Diisostearyl Trimethylolpropane Siloxy Silicate:</b> Substantive emollient,	5-
10%	
film former, durability, compatibility with organics, non-migrating	
<b>Alkyl Silicone Waxes:</b> Emollient, moisturizer "silicone petrolatum,"	
1-5%	
compatible with organics, thickener	



## GE Silicones

### Shampoo Components

- Cleansing Systems**
  - Detergents: Lauryl Sulfates, Laureth Sulfates, Sulfosuccinates, Betains, Sarcosinates
  - Foam Boosters: Amidoamines, Cocamide MEA, DEA, TEA, Amine Oxides, Polyols
- Conditioning Systems**
  - Oils: Mineral oil, Dimethicone, Cyclomethicone, Amodimethicone, Lanolin, Fatty Alcohols
  - Cationic Additives: Quats -Tricetylimonium Chloride, Cetrimonium Chloride. Polymers, Amodimethicone, Quaternium-10, -26, Jaguar
  - Viscosity Control Agents
  - Thickeners: Salt, Gums, Cellulose Derivatives, Synthetics, pH Adjusters
  - Thinner: Salt, Alcohol, Glycols, pH Adjusters, "Dimethicone Copolyols"
- Performance Enhancers**
  - Moisturization (for damaged hair): Dimethiconol emulsions, Amodimethicone
  - Volumizing (for fine hair): Silicone resins, Dimethiconol emulsions
  - Color retention (for color treated hair): Amodimethicone microemulsion
  - Frizz control: dimethicone
  - Fast Drying Time (less damage): Dimethiconol, Amodimethicone
- Preservative Systems**
- Additives**
  - Opacifiers, Pearlescing Agents, Fragrances, Colorants



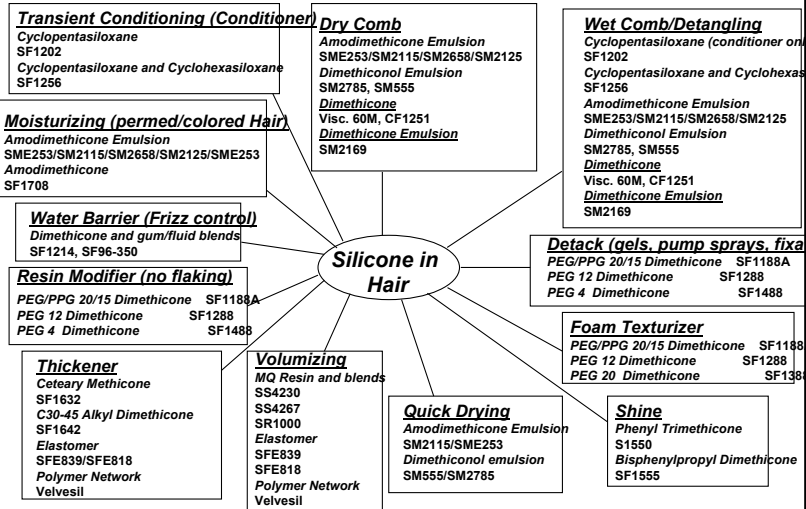
### Hair Fiber Properties Modified by Silicones

- **Frictional:** affects combability, feel, body, and hair breakage
- **Electrostatic:** affects triboelectric charging, or Fly-away
- **Visual:** affects appearance- luster, gloss, shine, oiliness
- **Wettability:** affects spreading of water and sebum
- **Resistance to Surface Abrasion:** affects surface wear
- **Interfiber Adhesion:** affects hair body and appearance



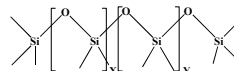
### Conditioner Attributes

- Detangle hair after shampooing
- Reduce combing forces for wet and dry hair
- Reduce fly-away
- Improves luster
- Makes hair manageable
- Impart softness
- Adjust pH of hair (after alkaline treatment)
- Temporarily mend split-ends
- Protect hair surface from wear (prevent breakage)
- Reduce drying time

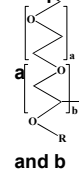


### Water-in-Silicone Emulsification Vehicle

INCI: Cyclopentasiloxane (and) Dimethicone Copolyol



Properties



Structure flexibility: x, y, a, b determine Physical

Water solubility: small x, large Y and

Organic solubility: small x, large Y

Diverse Product Possibility



**Water-in-Silicone Emulsification Vehicle**

*Cyclomethicone (and) Dimethicone Copolyol*  
*Cyclopentasiloxane (and) Dimethicone Copolyol*

- Effective in Stabilizing High Internal Phase Emulsions
- Unique Emulsifier allows Excellent Stability at Low Concentrations
  - Emulsifier Lowers interfacial tension
  - Forms boundary barrier, providing stability
  - Smooths out gradient between phases
- Ambient Processing Possible
- Clear Products by Refractive Index Matching
- Excellent Stability
- Non-greasy, Soft feel

**Water-in-Silicone Emulsification Vehicle  
SF1528****Typical Properties\***

INCI Name:	Cyclopentasiloxane (& Dimethicone Copolyol
Solids:	10-11%
Diluent/Carrier:	D <sub>5</sub>
Viscosity (25°C):	20-1,000 cP
Refractive Index (20°C):	1.3995-1.4015

\* Not intended to be specifications

**Antiperspirant Gel Formulation**

<u>Part A</u>	Wt%
Cyclopentasiloxane (SF1202)	10
Cyclopentasiloxane (& Dimethicone Copolyol (SF1528)	10

<u>Part B</u>	
Rezal 36G (46% salt)	44.5
DI Water	2.5
Propylene glycol	25.5
Ethanol	7.5

**Multifunctional Silicone Formulation Matrix**

**INCI Name:** Cyclopentasiloxane (& Dimethicone/Vinyl Dimethicone Crosspolymer

**Japan:** Decamethylcyclopentasiloxane CLSS 520778 (& Crosslinked Methylpolysiloxane CLSS 523061

**Functions:**

- **Emollient**
- **Sensory Modifier**
- **Thickener**
- **Stabilizer**
- **Delivery System for Actives**
- **Patented Technology**

**SFE839 Physical Properties**

Appearance:	Clear Colorless Gel
Silicone Solids:	5.25-5.75
Worked Viscosity *(25°C, cP):	10,000-30,000
Specific Gravity (25°C):	0.95
Density (lb/gal):	7.98
Flash Point (Closed Cup, °C)	82
Freezing Point (°C)	-44

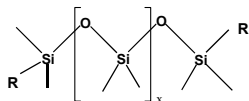
**Silicone Elastomer Dispersion**

Cyclopentasiloxane (&amp; Dimethicone/Vinyl Dimethicone Crosspolymer)

- **Unique Sensory Properties:** Dry, Powdery, Lubricious, Cushioning, Easily Absorbed
  - Application emolliency: related to spreading ease
  - Residual emolliency: related to lubricity
- **High Efficiency Thickener** for low silicones and esters
- **Stabilizer and Formulation Matrix** for Anhydrous Systems
  - No or minimal syneresis
  - Low solid --> Minimal interference, better efficacy for active ingredients
- **Cold/Ambient Processing**
- **Hydrophobic, Improve Wash-off Resistance and Durability**

**ALKYL MODIFIED SILICONE WAX**

INCI Name: C30-45 Alkyl Dimethicone

R = C<sub>30-45</sub> Alkyl

High melting point: 60-70 °C

Structuring agent for silicones

Minimal syneresis for anhydrous systems

Enhanced stability for emulsions

Superior compatibilizing agent for silicones and organic ingredients

Pastilled form for ease of handling

**Alkyl Modified Silicone Wax**

INCI Name: C30-45 Alkyl Dimethicone

**Physical Properties:**

Appearance:	Off-white pastille
Melting Point (°C):	60-70
Density lb/gal (25°C):	7.35
Compatibility:	Compatible with Organic waxes Compatible with Silicones



Hydrocarbons and Vegetable Oils

Mineral oil 65/75 SUS	SH
Mineral oil 200/210 SUS	SH
Petrolatum	SH
Cotton Seed Oil	SH
Castor Oil	IH
Sunflower Seed Oil	PSH
Maleated Soybean Oil	PSH
Wheat Germ Oil	IH
Hydrogenated Polyisobutene	SH
Isododecane	SH

Sunscreens

Octocrylene	IH
Oxybenzone	IH
Octyl Methoxycinnamate	PSH
Octyl Salicylate	SH

Alcohols and Glycols

Cetyl Alcohol	SH
Ethanol	I
SD Alcohol 40	I
Isopropanol	I
2-Ethyl-Hexanol	SH
Lauryl Alcohol	SH
Stearyl Alcohol	SH
Propylene glycol	PSH
Glycerin	IH

Other and Pigment

Tocopheryl Acetate	SH
Titanium Dioxide	DH
D&C Red #21	DH
Iron Oxide	DH

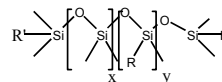
SF1642 Compatibility

Esters	
Isopropyl Palmitate	SH
Isopropyl Myristate	SH
Myristyl Propionate	SH
PPG-2 Myristyl Ether Propionate	SH
Caprylic/Capric Triglyceride	SH
C12-15 Alkyl Benzoate	SH
Silicones	
Dimethicones(SF96-350)	PSH
Cyclopentasiloxane(SF1202)	SH
Cyclopentasiloxane (and) Trimethylsilyloxylicilate (SS4230)	SH
Diisostearyl Trimethylolpropane Siloxy Silicate(SF1318)	PSH
Dimethicone Copolyol (SF1288)	PSH
Pheryl Trimethicone(SF1550)	SH
Bis-Phenylpropyl Dimethicone (SF1555)	SH
Waxes	
Paraffin	SH
Ozokerite	SH
Candelilla Wax	SH
Beeswax	SH
Carnauba	SH

I = Insoluble at <1%  
 IH = Insoluble Hot at <1%  
 SH = Soluble Hot at 10% or higher  
 PSH = Partially Soluble Hot at 1-10%  
 DH = Dispersible hot



Bis-Phenylpropyl Dimethicone: SF1555



R<sup>1</sup> = Phenylpropyl

Viscosity @ 25°C: 12 cS  
 Non-irritating  
 Refractive Index: 1.46  
 Low Odor  
 Non Greasy

APPLICATION BENEFITS

- Cuticle Coat
- Spray-on Gloss Products
- Skin Care
- Cosmetics
- AP/DEO

Sheen/gloss, compatibility  
 Sheen/gloss, compatibility  
 Compatible with organic ingredient and sunscreens  
 Non-greasy, Non-oily, Detackify, Emollient  
 Compatible with organic ingredients  
 Hydrophobic, Long lasting  
 Low residue; raise oil phase refractive index for clear gels



Hydrocarbons and Vegetable Oils

Mineral oil 65/75 SUS	S
Mineral oil 200/210 SUS	S
Petrolatum	SH
Cotton Seed Oil	S
Castor Oil	I
Sunflower Seed Oil	S
Maleated Soybean Oil	S
Wheat Germ Oil	S
Hydrogenated Polyisobutene	S
Isododecane	S

Sunscreens

Octocrylene	S
Oxybenzone	PSH
Octyl Methoxycinnamate	S
Octyl Salicylate	S
Octyl Dimethyl PABA	S

Alcohols and Glycols

Cetyl Alcohol	SH
Ethanol	PS
SD Alcohol 40	PS
Isopropanol	PS
Lauryl Alcohol	S
Stearyl Alcohol	SH
Propylene glycol	I
Butylene Glycol	I
Glycerin	I

Other and Pigment

Tocopheryl Acetate	S
Titanium Dioxide	D
D&C Red #21	D
Iron Oxide	D

SF1555 Compatibility

Esters	
Isopropyl Palmitate	S
Isopropyl Myristate	S
Octyl Dodecyl Neopentanoate	S
PPG-2 Myristyl Ether Propionate	S
C12-15 Alkyl Benzoate	S
Silicones	
Dimethicones(SF96-350)	PS
Cyclopentasiloxane(SF1202)	S
Cyclopentasiloxane (and) Trimethylsilyloxylicilate (SS4230)	S
Diisostearyl Trimethylolpropane Siloxy Silicate(SF1318)	S
Dimethicone Copolyol (SF1288)	S
Pheryl Trimethicone(SF1550)	S
Cetearyl Methicone (SF1632)	SH
C30-45 Alkyl Dimethicone (SF1642)	SH
Trimethylsilylamodimethicone (SF1708)	S
Waxes	
Paraffin	SH
Ozokerite	SH
Candelilla Wax	SH
Beeswax	SH
Carnauba	SH

I = Insoluble at <1%    D = Dispersible at 90%  
 S = Soluble at > 10%    PS = Partially Soluble at 1-10%  
 SH = Soluble Hot at 10% or higher  
 PSH = Partially Soluble Hot at 1-10%



Sunscreen with SFE839, SF1642 and Physical UV Absorber

Oil Phase

Cyclopentasiloxane & Dimethicone Copolyol (SF1528)	8.0	10.0 wt.%
Cyclopentasiloxane (SF1202)	10	16.0
Cyclopentasiloxane & Dimethicone/ Vinyl dimethicone Crosspolymer (SFE839)	10	3.0
Sorbitan Oleate	0.5	0.5
C30-45 Alkyl Dimethicone (SF1642)	2.0	1.0
Microfine TiO <sub>2</sub> (Hydrophobic) <sup>1</sup>	5.0	5.0

Water Phase

Sodium Chloride	0.2	0.2
Water	59.3	61.9
Butylene Glycol	-	2.0
Preservative	q.s.	q.s.

1: UV-Titan X161, Presperse Inc.



**Water-in-Oil Sunscreen with SFE839, SF1555 and SF1642**

<b>Component</b>	<b>Wt. %</b>
<i>Oil Phase</i>	
Cyclopentasiloxane (&) Dimethicone Copolyol (SF 1528)	10.0
Octyl Methoxy Cinnamate	7.5
Octyl Salicylate	3.0
Oxybenzone	3.0
Cyclopentasiloxane (and) Dimethicone/ Vinyl dimethicone Crosspolymer (SFE839)	5.0
Bis-Phenylpropyl Dimethicone (SF1555)	5.0
C30-45 Alkyl Dimethicone (SF1642)	1.0
Sorbitan Oleate	0.5
<i>Water Phase</i>	
NaCl	0.5
Water	64.5
Preservative and Fragrance	q.s.

Formulation stability has not been established