Final Report

On the Safety Assessment of Ammonium Hectorites as Used in Cosmetics

March 16, 2012

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ABSTRACT: The CIR Expert Panel reviewed the safety of 4 ammonium hectorite compounds used in cosmetics: disteardimonium hectorite, dihydrogenated tallow benzylmonium hectorite, stearalkonium hectorite, and quaternium-18 hectorite. These ingredients function in cosmetics mainly as nonsurfactant suspending agents. The Panel reviewed available animal and human data related to these ingredients. The Panel concluded that these ammonium hectorite compounds were safe as cosmetic ingredients in the practices of use and concentration as given in this safety assessment.

INTRODUCTION

This report assesses the safety of ammonium hectorites as used in cosmetics. The ingredients in this report are: disteardimonium hectorite, dihydrogenated tallow benzylmonium hectorite, stearalkonium hectorite, and quaternium-18 hectorite. These ingredients function in cosmetics mainly as suspending agents – nonsurfactant.

Stearalkonium hectorite and quaternium-18 hectorite have been reviewed by the CIR Expert Panel and were found to be safe for use in cosmetics.[1,2] Summaries of the relevant data from these reports are summarized below in the appropriate sections.

The silicate clay hectorite were previously reviewed by the CIR Expert Panel as part of a group of alumninum silicate clays and found to be safe as used in cosmetic products.[3] Quaternium-18 was also previously reviewed and was found to be safe as a cosmetic ingredient.[1]

CHEMISTRY

Definition and Structure

Hectorite is part of a group of phyllosilicate, layered, clay-based minerals, the general term for which is smectites, the most prominent of which are montmorillonite, beidellite, nontronite, saponite and hectorite.[4] Hectorite and montmorillonite were included in the previous safety assessment of silicate clays. [3] These various clays are differentiated by variations in chemical composition involving substitutions of aluminum for silicon in tetrahedral cation sites and aluminum, iron, magnesium and lithium in octahedral cation sites.

Smectite minerals have a variable net negative charge, which is balanced by sodium, calcium, or magnesium ions adsorbed externally on interlamellar surfaces. The structure, chemical composition, exchangeable ion type and small crystal size of smectite minerals are responsible for several unique properties, including a large chemically active surface area, a high cation exchange capacity, interlamellar surfaces having unusual hydration characteristics, and the ability to modify strongly the flow behavior of liquids. In the cosmetics industry, clay based products are used to improve properties such as suspension, emulsion stability, viscosity, thermal stability and spreadability.

Structurally, hectorite is a trioctahedral, magnesium/lithium silicate based mineral that is amorphous and does not contain any crystalline silica. In the previous safety assessment of silicate clays, hectorite was given as containing fluorine, [3] but current information suggests that was not correct.

Because of isomorphous substitution of lithium ions (a plus one charge) for magnesium ions (a plus two charge) in the octahedral sheet during hectorite formation, the surfaces of these minerals have a delocalized net negative charged in the lattice.[5] Cations located between two consecutive layers (octahedral sheets) contribute to compensate the structural charge and to keep the layers bound. Thus, cations like sodium are attracted to the mineral surface to counterbalance the interlayer charge. These cations can easily be exchanged, since they are retained by electrostatic attractions.

Organo-hectorite minerals, such as disteardimonium hectorite, stearalkonium hectorite, quaternium-18 hectorite, and dihydrogenated tallow benzylmonium hectorite are synthesized by grafting cationic surfactants to hectorite (i.e., exchanging the interlayer sodium cations with a cationic surfactant). These cationic surfactants are quaternary ammonium compounds with the template formulae $[(CH_3)_3NR]^+$, $[(CH_3)_2NRR']^+$, and $[CH_3NRR'R'']^+$, wherein R, R', and R" are alkyl or aromatic hydrocarbons. For instance, in the case of disteardimonium hectorite at least some of the sodium cations of hectorite have been exchanged for the $[(CH_3)_2NRR']^+$ cation, wherein R and R' are both octadecyl alkyl chains (i.e., stearyl groups). The exchange is typically carried out by the addition of the appropriate ammonium chloride (e.g., disteardimonium chloride) to an alcohol/water slurry of hectorite.[6,7] The major byproduct therein is sodium chloride, which is removed during processing (Figure 1). This cation exchange shifts the nature of these minerals from hydrophilic to lipophilic.[6,7]

Physical and Chemical Properties

The physical and chemical properties of the ingredients in this safety assessment are provided in Table 2.

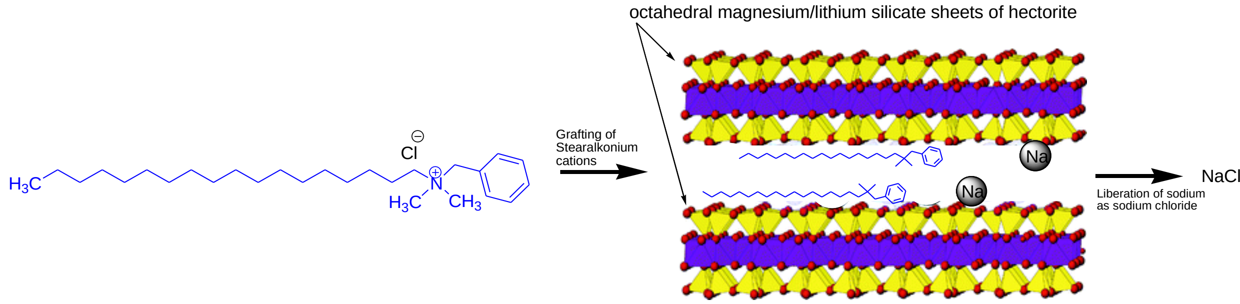


Figure 1. Synthesis of organo-clay minerals.

Hectorite

The unique physicochemical properties of smectite clays, including hectorite, are the result of (i) extremely small crystal size, (ii) variations in internal chemical composition, (iii) structural characteristics caused by chemical factors, (iv) large cation exchange capacity, (v) large surface area that is chemically active, (vi) variations in types of exchangeable ions and surface charge, and (vii) interactions with inorganic and organic liquids.[4]

Because of aggregation, the effective particle size will be larger and the surface area considerably less than the actual particle size and surface area. During the growth of hectorites, by either transformation or neoformation, crystals become interlocked and become difficult to separate except by a strong shearing force. Differences in the effective particle size of hectorites are extremely important in the determination of properties such as ion exchange, viscosity and fluid loss.[4,8]

QUATERNIUM-18 HECTORITE

Quaternium-18 hectorite is reported to be an inert, chemically stable material. It is pH and heat stable under normal cosmetic use conditions.[9,10]

Impurities

QUATERNIUM-18 HECTORITE

Methyl ditallow amine, methyl ditallow ammonium hectorite, and sodium chloride are possible impurities in quaternium-18 hectorite.[11]

STEARALKONIUM HECTORITE

Stearalkonium hectorite contains a maximum of 3 ppm and 20 ppm elemental arsenic and elemental lead, respectively.[12] Sodium chloride may be formed during the ionic exchange reaction of stearalkonium chloride and hectorite, which is washed out down to < 0.5%. "Adsorbed" cations were between 3.0% and 5.0% on stearalkonium hectorite.

USE

Cosmetic

Data on ingredient usage are provided to the Food and Drug Administration (FDA) Voluntary Cosmetic Registration Program (VCRP) and a survey conducted by the Personal Care Products Council (Council) collected maximum use concentrations for ingredients in this group.[13-15] The VCRP reported that disteardimonium hectorite was used in 574 leave-on products (maximum of 28% in makeup preparations) and 10 rinse-off products (maximum of 4% in hair coloring preparations; Table 4). Quaternium-18 hectorite was reported to be used in 106 leave-on products (maximum of 5% in mascara) and 5 rinse-off products (no concentrations of use for his category was reported by the Council). Stearalkonium hectorite was used in 467 leave-on products (maximum of 6% in nail polishes and enamels) and 2 rinse-off products (maximum of 3% in eye makeup remover). Of the 467 leave-on products, 277 were in nail polish and enamels. There were no reported uses of dihydrogenated tallow benzylmonium hectorite.

Non-Cosmetic

Quaternium-18 hectorite is used as a dispersant in volatile oils.[16] It has also have been tested as granulators and binders in the production of tablets.

TOXICOKINETICS

Absorption, Distribution, Metabolism, and Excretion

There were no studies on absorption, distribution, metabolism or excretion discovered.

TOXICOLOGICAL STUDIES

Acute Toxicity

Dermal

There were no acute dermal toxicity studies discovered for these cosmetic ingredients.

Oral – Non-Human

QUATERNIUM-18 HECTORITE

The oral LD_{50} of quaternium-18 was > 10 g/kg for rats.[17]

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

The oral LD_{50} for dihydrogenated tallow benzylmonium hectorite was > 5.0 g/kg for Spargue-Dawley rats (n = 1-).[18]

Inhalation – Non-Human

QUATERIUM-18 HECTORITE

Aerosolized quaternium-18 hectorite (202 mg/L in isopropyl myristate) was not toxic to rats (n = 10) after 1 h.[7,17]

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

The inhalation LC_{50} for dihydrogenated tallow benzylmonium hectorite was > 5.2 mg/L for Spargue-Dawley rats (n = 5/sex) after 4 h.[18]

Repeated Dose Toxicity

Dermal – Non-Human

QUATERNIUM-18 HECTORITE

Quaternium-18 hectorite (up to 50%) applied, unoccluded, to the exposed skin of rabbits 3x/d for 5 days/week for 3 weeks caused no toxic effects.[7,17] There was mild drying and scaling of the upper layers of the skin during the early days of the study.

STEARALKONIUM HECTORITE

There were no toxic effects observed when stearalkonium hectorite was dermally applied to rabbits twice per day, unoccluded, at concentrations of 12.5% to 50% over 3 weeks.[19]

REPRODUCTIVE AND DEVELOPMENTAL TOXICITY

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

Orally administered dihydrogenated tallow benzylmonium hectorite had a no effect level of 1000 mg/kg to Sprague-Dawley rats.[20] The test material was administered throughout the complete reproductive cycle for 1 generation.

GENOTOXICITY

In Vitro

STEARALKONIUM HECTORITE

Stearalkonium hectorite was not mutagenic to *Salmonella typhimurium* (TA98, TA100, TA1535, TA1537 and TA1538) up to 1500 µl/plate or mouse lymphoma cells up to 500 µl/plate.[21,22]

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

Dihydrogenated tallow benzylmonium hectorite (concentration not provided) was not mutagenic in an Ames test using *Salmonella* with or without metabolic activation.[20]

CARCINOGENICITY

There were no carcinogenicity studies discovered for these cosmetic ingredients.

IRRITATION AND SENSITIZATION

Irritation

Dermal – Non-Human

QUATERNIUM-18 HECTORITE

Quaternium-18 hectorite (50%) was not dermally irritating to rabbits.[17]

STEARALKONIUM HECTORITE

Stearalkonium hectorite (50% w/v in water with 2.5% polysorbate 809) did not cause erythema or edema to albino rabbits.[19]

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

Dihydrogenated tallow benzylmonium hectorite (0.5 g in 0.5 mL saline) was not irritating when administered to the intact and abraded skin of New Zealand White rabbits (n = 6) for 24 h.[20]

Dermal – Human

DISTEARDIMONIUM HECTORITE

A patch test of a cosmetic mixture product containing disteardimonium hectorite (15% with cyclomethicone and PEG-10 dimethicone[23]; diluted to 1.5% in mineral oil) was conducted on female subjects (n = 11) of various skin types.[24] The occlusive patches were left in place for 48 h. The test site was examined at patch removal and 15 min later. There were no signs of irritation observed.

A patch test of a cosmetic mixture product containing disteardimonium hectorite (15%) was conducted on subjects (n = 10).[25] The patches were left in place for 24 h and the test sites observed at removal and after 24 h. There were no signs of irritation observed.

STEARALKONIUM HECTORITE

Stearalkonium hectorite (50% w/v in water with 2.5% polysorbate 809; n = 50) was not irritating in a repeated insult patch test (100%) or in a facial mask containing stearalkonium hectorite (1.4%; n = 27).[26,27]

Ocular

QUATERNIUM-18 HECTORITE

Quaternium-18 hectorite (50%; 0.1 ml) was not irritating to rabbits.[7]

Quaternium-18 hectorite (2 mg neat; 20g in 100 ml physiological saline or corn oil) instilled in the eyes of subjects did not cause any abnormal ocular sensations.[17] No pain was reported. A "sand-like" feeling was reported in the saline sample. No damage to the eye was observed.

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

Dihydrogenated tallow benzylmonium hectorite (0.5 g in 0.5 mL saline) was practically non-irritating when administered to the eyes of New Zealand White rabbits (n = 6 rinsed after 4 sec; n = 3 not rinsed).[20]

STEARALKONIUM HECTORITE

Stearalkonium hectorite (up to 100%; volumes not provided) was a minimal to mild ocular irritant to rabbits.[7,28] In an Eyetex in vitro test of products, an eyeliner containing stearalkonium hectorite (0.196%;), a lipliner pencil (1.0%), and a face mask (5.0%) were classified as minimal to mild irritants.[29]

Sensitization

Dermal – Non-human

DIHYDROGENATED TALLOW BENZYLMONIUM HECTORITE

It was reported that dihydrogenated tallow benzylmonium hectorite (concentration not provided) did not cause delayed contact hypersensitivity in albino guinea pigs (n not provided).

Dermal – Human

QUATERNIUM-18 HECTORITE

Quaternium-18 hectorite (100%) was not irritating or sensitizing in a repeated insult patch test (n = 50).[20]

Quaternium-18 hectorite was not sensitizing in an eye shadow (n = 50), a blusher (n = 209), and 3 undisclosed products (n – 12) up to 10%.[17,30]

DISTEARDIMONIUM HECTORITE

A human repeated insult patch test (HRIPT; n = 112) was conducted on disteardimonium hectorite (100%; 20 μg) using an occlusive Finn chamber.[31] The test material was not sensitizing.

STEARALKONIUM HECTORITE

Stearalkonium hectorite (50% w/v in water with 2.5% polysorbate 809) was not sensitizing in a repeated insult patch test (n = 50) or in a product containing stearalkonium hectorite (1.4%).[26]

SUMMARY

Ammonium hectorites are a group of ingredients that function in cosmetics mainly as nonsurfactant suspending agents. The ingredients in this report are: disteardimonium hectorite, dihydrogenated tallow benzylmonium hectorite, stearalkonium hectorite, and quaternium-18 hectorite.

Hectorite is a trioctahedral, magnesium/lithium silicate based mineral that is amorphous and does not contain any crystalline silica. The relatively weak electrostatic interactions of thin crystalline layers can essentially be 'propped open' to allow the insertion of certain molecules and atoms (i.e., disteardimonium, quaternium-18).

Disteardimonium hectorite was used in 574 leave-on products up to 28% and 10 rinse-off products up to 4%. Stearalkonium hectorite was used in 467 leave-on products up to 6% and 2 rinse-off products up to 3%. Quaternium-18 hectorite was reported to be used in 106 leave-on products up to 5% and 5 rinse-off products.

The oral LD_{50} for dihydrogenated tallow benzylmonium hectorite was 5.0 g/kg for rats. The oral LD_{50} of quaternium-18 was > 10 g/kg. The inhalation LC_{50} for dihydrogenated tallow benzylmonium hectorite was > 5.2 mg/L for rats after 4 h. Aerosolized quaternium-18 hectorite was not toxic to rats at 202 mg/L after 1 h.

Stearalkonium hectorite was not dermally toxic to rabbits at concentrations of 12.5% to 50% over 3 weeks.

Quaternium-18 hectorite applied to the exposed skin of rabbits for 3 weeks was not toxic up to 50%.

Stearalkonium hectorite was not mutagenic to *Salmonella typhimurium* up to 1500 µl/plate or mouse lymphoma cells up to 500 µl/plate.

Stearalkonium hectorite did not cause erythema or edema to albino rabbits at 50% w/v. Quaternium-18 hectorite (50%) was not irritating to rabbits. Dihydrogenated tallow benzylmonium hectorite at 0.5 g in 0.5 mL saline was not irritating when administered to the intact and abraded skin rabbits.

Disteardimonium hectorite was not irritating to humans in 2 patch tests at 15%. Stearalkonium hectorite was not irritating or sensitizing to humans at 100%. Dihydrogenated tallow benzylmonium hectorite (concentration not provided) did not cause delayed contact hypersensitivity in albino guinea pigs.

Stearalkonium hectorite was a minimal to mild ocular irritant to rabbits and human subjects. It was classified as a minimal to mild irritant in 3 in Eyetex in vitro tests of products. Quaternium-18 hectorite was not an ocular irritant at 50% in rabbits and at 2 mg in human subjects. Dihydrogenated tallow benzylmonium hectorite at 0.5 g in 0.5 mL saline was practically non-irritating when administered to the eyes of rabbits.

Quaternium-18 hectorite was not irritating or sensitizing up to 100% in HIPTs.

DISCUSSION

Single-dose toxicity data were available for quaternium-18 hectorite and dihydrogenated tallow benzylmonium hectorite, and repeated-dose toxicity data were available for quaternium-18 hectorite and stearalkomonium hectorite. Genotoxicity data were available for stearalkomonium hectorite and dihydrogenated tallow benzylmonium hectorite, and reproductive and developmental toxicity data were available for dihydrogenated tallow benzylmonium hectorite. Irritation and sensitization data were available for all of these ingredients. Overall, no significant toxicity was reported and these ingredients were not dermal irritants or sensitizers. The CIR Expert Panel considered that the chemical structures of these clay-based ingredients were sufficiently similar, as was the pattern of use in cosmetics, to support using data on each individual ingredient to support the safety of the entire group.

The Panel noted that the hectorites in this safety assessment have high chemical stability and are biochemically inert. The Panel considered the lithium substitution for magnesium in the magnesium/lithium silicate sheet structure, but concluded lithium is tightly bound and not likely to leach. The substitution of lithium for magnesium at many sites in the lattice structure gives the material a delocalized net negative charge in the lattice. While no data were available on dermal penetration, the Panel considered that the charge properties and the large molecular weight of these clay-like ingredients would preclude significant dermal penetration. Because they are chemically inert, no metabolites are expected that would penetrate the skin.

CONCLUSION

The CIR Expert Panel concluded that disteardimonium hectorite, dihydrogenated tallow benzylmonium hectorite, stearalkonium hectorite, and quaternium-18 hectorite are safe in the present practices of use and concentration described in this safety assessment. Were dihydrogenated tallow benzylmonium hectorite (not in current use) to be used in the future, the expectation is that it would be used in product categories and at concentrations comparable to others in this group.

TABLES AND FIGURES

Table 1. Definitions of ammonium hectorite ingredients as in the *International Cosmetic Ingredient Dictionary and Handbook* followed by the definition developed by the CIR staff (in *italics*).[32]

Ingredient CAS No.	Definition	Function
Quaternium-18 hectorite 12001-31-9 71011-27-3	Quaternium-18 hectorite is a reaction product of hectorite and quaternium-18. *Quaternium-18 hectorite is the cation exchange product of hectorite and quaternium-18. Essentially, some of the sodium cations of hectorite are replaced with di(hydrogenated tallow)dimethylammonium cations.*	Suspending Agents - Nonsurfactant
Disteardimonium hectorite 94891-31-3 [CAS No. reflects diceteardimonium hectorite; i.e. di-C16-18 dimethyl-ammonium hectorite]	Disteardimonium hectorite is the reaction product of distearyldimonium chloride and hectorite. *Disteardimonium Hectorite is the cation exchange product of distearyldimonium chloride and hectorite. Essentially, some of the sodium cations of hectorite are replaced with distearyldimethylammonium cations.*	Suspending Agents - Nonsurfactant
Stearalkonium hectorite 12691-60-0 94891-33-5	Stearalkonium hectorite is a reaction product of hectorite (q.v.) and stearalkonium chloride. *Stearalkonium hectorite is a cation exchange product of hectorite and stearalkonium chloride. Essentially, some of the sodium cations of hectorite are replaced with benzyldimethylstearylammonium cations.*	Suspending Agents - Nonsurfactant
Dihydrogenated tallow benzylmonium hectorite	Dihydrogenated tallow benzylmonium hectorite is the reaction product of hectorite and a dihydrogenated tallow benzyl monomethyl quaternary ammonium salt. *Dihydrogenated tallow benzylmonium hectorite is the cation exchange product of Hectorite and a di(hydrogenated tallow) benzyl monomethyl quaternary ammonium salt. Essentially, some of the sodium cations of hectorite are replaced with di(hydrogenated tallow)benzylmethylammonium cations*.	Suspending Agents - Nonsurfactant; Viscosity Increasing Agents - Aqueous; Viscosity Increasing Agents - Nonaqueous

Table 2. Chemical and physical properties.

Property	Value	Reference
Disteardimonium hectorite		
Physical Form	Organically modified hectorite/Finely divided powder	33
Color	Creamy white	33
Density/Specific Gravity @ °C	1.7	33
Dihydrogenated tallow benzylmonium hectorite		
Physical Form	Smectite clay/finely divided powder	18
Color	Very light cream	18
Density/Specific Gravity @ °C	1.59	18
Stearalkonium Hectorite		
Physical Form	Fine powder	11
Color	Creamy White	11
Quaternium-18 hectorite		
Physical Form	Powder	16,34
Color	White, light cream-colored	16,34
Odor	Faint	34
Water Solubility g/L @ °C & pH	Insoluble	34

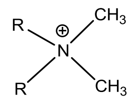
Table 4. Current Frequency and Concentration of Use According to Duration and Type of Exposure. There were no reported uses of dihydrogenated tallow benzylmonium hectorite.[13-15]

	Disteardimonium hectorite		Stearalkonium hectorite		Quaternium-18 hectorite	
	# of Uses	**Concentration (%)**	**# of Uses**	**Concentration (%)**	**# of Uses**	**Concentration (%)**
Duration of Use						
Totals*/Conc. range**	584	0.04-28	469	0.006-6	111	0.05-5
Leave-on	574	0.04-28	467	0.006-6	106	0.05-5
Rinse-off	10	0.7-4	2	3	5	NR
Diluted for (bath) use	NR	3	NR	NR	NR	NR
Exposure Type						
Eye area	202	0.02-15	40	0.2-3	42	1-5
Incidental ingestion	159	0.04-9	79	2-3	21	0.05
Incidental inhalation sprays	6	0.1-2	5	0.2-1[2]	6	0.02-3
Incidental inhalation powders		2	NR	NR	NR	NR
Dermal contact	329	0.07-28	84	0.006-3	68	0.02-3
Deodorant (underarm)	5	0.5-2[1]	NR	0.4[3]	4	0.02-3[4]
Hair – non coloring	1	0.3	1	NR	3	NR
Hair - coloring	NR	3-4	NR	NR	NR	NR
Nail	NR	NR	304	0.3-6	NR	NR
Mucous Membrane	160	0.04-9	81	2-3	23	0.05
Baby products	NR	NR	NR	NR	NR	NR

NR = Not Reported; Totals = Rinse-off + Leave-on Product Uses.
[1] 0.5%-2% in aerosol sprays, 4% in non-spray products.
[2] 0.3% in a body and hand spray
[3] 0.4% in both aerosol and pump sprays.
[4] 0.2%-3% in aerosol sprays.
Note: Because each ingredient may be used in cosmetics with multiple exposure types, the sum of all exposure type uses may not equal the sum total uses.

Figure 2. Structures/Formulas of ammonium hectorite ingredients.

Quaternium-18 Hectorite



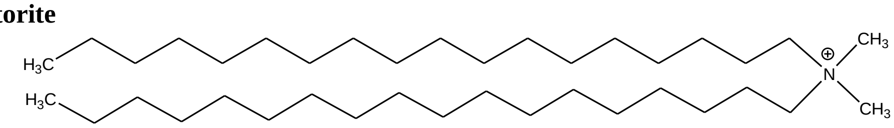
Dihydrogenated Tallow Dimonium cation: wherein R is the fatty acid chain residue of tallow

Hectorite formula: $Na_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Quaternium-18 Hectorite formula: $[Na,((CH_3)_2NR_2)]_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Disteardimonium Hectorite

Disteardimonium cation:

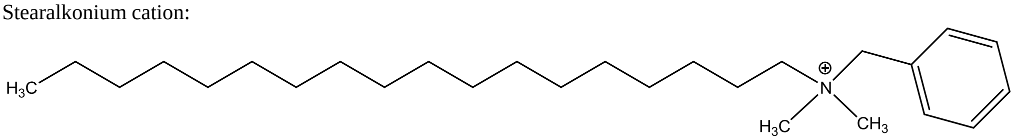


Hectorite Formula: $Na_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Disteardimonium Hectorite formula: $[Na,((CH_3)_2N((CH_2)_{17}CH_3)_2)]_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Stearalkonium Hectorite

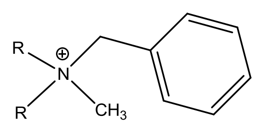
Stearalkonium cation:



Hectorite Formula: $Na_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Stearalkonium Hectorite formula: $[Na,((CH_3)_2N(CH_2)_{18}CH_3)(CH_2C_6H_5))]_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Dihydrogenated Tallow Benzylmonium Hectorite



Dihydrogenated Tallow Benzylmonium cation: wherein R is the fatty acid chain residue of tallow

Hectorite Formula: $Na_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

Dihydrogenated Tallow Benzylmonium Hectorite formula: $[Na,(CH_3NR_2(CH_2C_6H_5)]_{0.33}[Mg_{2.67},Li_{0.33}]Si_4O_{10}[OH]_2$

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