### SIDS INITIAL ASSESSMENT PROFILE

<table>
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<th>Chemical Category</th>
<th>Organoclays Category</th>
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<td><strong>CAS numbers and Chemical Names</strong></td>
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| **71011-26-2**: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite, (Benzyl monoalkyl chain quaternary ammonium compound \[B(Alk)2M\] hectorite). Same as CAS numbers 94891-33-5 and 12691-60-0. | The quaternary ammonium compounds (cations) have the following general formula: \( N^+ R_1 R_2 R_3 R_4 \) where \( R_1, R_2, R_3, \) and \( R_4 \) are substitutions on the N (nitrogen atom) of the quaternary compound (salt) as follows:  
- methyl – 1 or 2 substitutions  
- benzyl – 0 or 1 substitutions  
- alkyl (C\(_{14-22}\)) – 1, 2 or 3 substitutions  |
| **68953-58-2**: Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, salts with bentonite, (Dialkyl chain quaternary ammonium compound \(2M(2Alk)\) bentonite). Same as CAS numbers 1340-69-8 and 73138-28-0. | The clays (anions) are made of silicon, hydrogen and oxygen (hectorite, montmorillonite, smectite). |
| **71011-27-3**: Quaternary ammonium compounds, bis(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with hectorite, (Dialkyl chain quaternary ammonium compound \(2M(2Alk)\) hectorite). Same as CAS numbers 94891-31-3, 97280-96-1 and 12001-31-9. | **68153-30-0**: Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, chlorides, compounds with bentonite, (Benzyl dialkyl chain quaternary ammonium compound \[B(2Alk)M\] bentonite). Same as CAS numbers 121888-66-2 and 89749-77-9. |
| **71011-24-0, 71011-25-1, 121888-68-4 and 89749-78-0**: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite; (Benzyl monoalkyl chain quaternary ammonium compound \[B(Alk)2M\] bentonite). | **91080-57-8 and 91080-56-7**: Quaternary ammonium compounds, benzyl (hydrogenated tallow alkyl) dimethyl, chlorides, compounds with smectite (Benzyl monoalkyl chain quaternary ammonium compound \[B(Alk)2M\] smectite). Note that 91080-56-7 is [di-C\(_{10-C22}\) alkyl, dimethyl]. |
| **97952-68-6**: Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with montmorillonite, (Benzyl dialkyl chain quaternary ammonium compound \(B(2Alk)2M\) montmorillonite). | **68911-87-5**: Bis(hydrogenated tallow alkyl)dimethylammonium with montmorillonite (Dialkyl chain quaternary ammonium compound \(2M(2Alk)\) montmorillonite). |
| **71011-24-0, 71011-25-1, 121888-68-4 and 89749-78-0**: Quaternary ammonium compounds, benzyl(hydrogenated tallow alkyl)dimethyl, chlorides, compounds with bentonite; (Benzyl monoalkyl chain quaternary ammonium compound \[B(Alk)2M\] bentonite). | **91081-06-0**: Bis(hydrogenated tallow alkyl)dimethylammonium with smectite (Dialkyl chain quaternary ammonium compound \(2M(2Alk)\) smectite). Note this substance is [di-C\(_{10-C22}\) alkyl, dimethyl]. |
| **121888-67-3**: Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with hectorite (Benzyl dialkyl chain quaternary ammonium compound \[B(2Alk)M\] hectorite). | **97952-68-6**: Quaternary ammonium compounds, benzylbis(hydrogenated tallow alkyl)methyl, salts with montmorillonite, (Benzyl dialkyl chain quaternary ammonium compound \(B(2Alk)2M\) montmorillonite). |

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bentonite and smectite); and sodium, lithium, and magnesium, (hectorite); sodium, calcium, aluminum, magnesium (montmorillonite, bentonite); or aluminum (smectite).

SUMMARY CONCLUSIONS OF THE SIAR

Category Justification

A key factor supporting the grouping of compounds within the Organoclays Category is structural similarity. Four clays (bentonite, smectite, montmorillonite, and hectorite) are represented by the CAS numbers in this category. These clays are closely related and, in some cases, have been used interchangeably to describe structurally similar clay minerals. Bentonite is a naturally occurring material consisting predominantly of the clay mineral montmorillonite, which is in turn the family of sheet silicates called smectites. Hectorite is also included in the smectite group (along with stevensite and saponite). Deposits in which one of these clay minerals predominate are more commonly referred to by that clay mineral’s name. Thus, considering the similarity in the clay minerals of this category, the defining differentiation between the groups is the organic cation which is reacted with the clay.

All smectite clay minerals (which include hectorite and montmorillonite in this category) possess similar structural properties. They are two-dimensional inorganic polymers with a layered structure. Each individual crystal is one unit cell (or about one nanometer) thick, up to 1000 nanometers across, and carries a net negative charge typically between 0.8-1.5 meq/g. This charge attracts cations to the large exterior surfaces of the individual clay crystals. The sodium and calcium cations common in naturally-occurring smectites give the layer surfaces a strongly hydrophilic nature, and the calcium cation binds to the clay more tightly than the sodium cation. The cations can be readily exchanged with quaternary ammonium cations to produce the organoclay compounds. In contrast to the calcium and sodium cations, the quaternary ammonium ions are tightly held to the clay, resulting in organoclay compounds (“salts”) that are very hydrophobic in nature.

CAS numbers have been assigned in a way that suggests a category of many distinct compounds. The apparent complexity of this category results from (1) the same quaternary compound (salt) complexed with the three different clay types, and (2) the same alkyl (C14-22) moiety originating from different sources (tallow or vegetable oil).

Human Health

Based on the toxicokinetic data with B(Alk)2M bentonite, organoclay compounds are not expected to be absorbed following oral (gavage) exposure and will be excreted directly and rapidly in feces with negligible elimination via urine and bile. There is no evidence of any tissue retention or systemic uptake of these substances. Based on reported particle size distribution data for consumer and industrial products, these materials are not expected to be respirable. These materials are also not expected to be absorbed through the skin based on the physical chemical properties as well as these reported particle sizes.

Numerous acute toxicity studies have been conducted with all organoclay category members except B(2Alk)M monomorillonite. The studies show a low order of toxicity with inhalation 4-hr LC50s and oral (gavage) LD50s greater than 5.0 mg/L and 5,000 mg/kg bw, respectively. The inhalation 1 hr LC50 > 200 mg/L for B(Alk)2M hectorite. Common clinical signs associated with acute inhalation in several studies included transient weight loss and respiratory irregularity. Clinical signs observed in the oral studies included diarrhea, rapid breathing, piloerection, swollen abdomen, ataxia and lethargy. Acute dermal toxicity studies were not located for the organoclays. The organoclays are not irritating to the skin. Eye irritation is generally minimal in humans (irritation due to the physical nature of the compounds were noted), although observations of moderate irritation have been reported in animals. Skin sensitization tests conducted with 2M(2Alk) bentonite, and B(Alk)2M bentonite and B(2Alk)M hectorite indicate the organoclay materials are not sensitizers.

Repeated-dose toxicity studies by the oral route of exposure (gavage or dietary) and using methods similar to OECD TG 407 have been conducted with 2M(2Alk) bentonite, and B(Alk)2M bentonite and B(2Alk)M hectorite. The NOAEL for 2M(2Alk) bentonite in a 12-week rat dietary study was 25% (approx. 12,500-25,000 mg/kg-bw/day), the
highest dose tested. The NOAEL for B(Alk)2M bentonite in a 28-day rat oral (gavage) study was 1,000 mg/kg bw/d, the only dose tested. The LOAEL for B(2Alk)M hectorite in a 28-day rat oral (gavage) study was 1,000 mg/kg bw/d, the only dose tested based on decreased thrombotest time, decreased chloride and calcium levels, and increased adrenal weights. The repeated-dose toxicity of the remaining members of the Organoclays Category (B(Alk)2M hectorite, 2M(2Alk) hectorite, B(2Alk)M bentonite and B(2Alk)M montmorillonite) is expected to be similar.

The category members B(Alk)2M hectorite, 2M(2Alk) bentonite, and 2M(2Alk) hectorite were tested in bacterial reverse mutation assays (with and without metabolic activation) and B[Alk]2M hectorite was tested in vitro using mouse lymphoma cells; these substances were negative for gene mutations in these assays. B(Alk)2M bentonite, was also negative in a reverse mutation assay. In in vivo chromosomal aberrations and in vivo micronucleus assays, B[Alk]2M bentonite and B[2Alk]M hectorite were both negative for chromosomal aberrations. Further testing is not appropriate due to the physical chemical properties of these materials.

There are no data available regarding the carcinogenicity of these materials. The impurity, respirable crystalline silica, (which may be present at levels of 0.2% in B(Alk)2M hectorite; 0.1-5% in 2M(2Alk) bentonite; and 0.1-10% in B(2Alk)M bentonite) is considered a known human carcinogen (Group 1 according to IARC).

A one-generation reproduction study using B(2Alk)M hectorite at dose levels of 0, 50, 225, and 1,000 mg/kg bw/d has been conducted for the potential to cause developmental toxicity in rats. The compound was not found to be teratogenic, nor was there any reproductive toxicity at any dose level. Based on the lack of reproductive toxicity or developmental effects with B(2Alk)M hectorite, the sponsored organoclay materials are not expected to cause developmental toxicity or to demonstrate reproductive toxicity at doses up to 1,000 mg/kg bw/day.

**Environment**

Although there may be some degradation when subjected to extreme heat beginning at about 180ºC up to approximately 600ºC, the organoclays do not melt or boil. Organoclays are free flowing solid powders that are essentially insoluble in water, in organic solvents and in lipids, and have no volatility under ambient conditions. Vapor pressure is not relevant because all members of the category are powders and are not volatile. Since organoclays are essentially insoluble in both water and lipids, the partition coefficient cannot be accurately determined. Densities of the substances range from 1.4 to 1.8. Organoclays are not inherently explosive, nor are they oxidizers.

Organoclays are anticipated to be found primarily in soil or sediment, although it is possible that smaller particles will be suspended in water. Estimates of atmospheric photodegradation are also not relevant due to the nature of these compounds. Organoclays will not hydrolyze because they resist base or acid attack over a pH range of 3-11. Because of their physico-chemical nature the organoclays cannot be evaluated using EPIWIN for distribution among environmental compartments.

In three separate OECD TG 306 biodegradation tests using B(2Alk)M bentonite, biodegradation ranged from 4.7 to 33.4% in 28 days, depending on the test. Based on these data as well as the structural and chemical properties of these compounds, it is assumed that other organoclay category members will also show limited biodegradation. It should be noted that biodegradation relates only to the organic component of the organoclays (i.e. the alkyl quaternary ammonium salts).

Fish acute toxicity studies have been performed with B(Alk)2M bentonite. The 96-hr LC₅₀ was > ca. 500 mg/L (nominal) in freshwater rainbow trout. In a semi-static test with rainbow trout (*Oncorhynchus mykiss*), the 21-day LC₅₀ was >1.0 mg/L (nominal) for this substance.

Acute aquatic invertebrate tests have been conducted. The nominal EC₅₀ values for the water flea (*Daphnia magna*) were >100 mg/L (48 hrs) for the category member 2M(2Alk) bentonite, 300 mg/L (96 hrs) and < 500 mg/L (48 hrs) for B(Alk)2M bentonite, and >100 mg/L (96 hrs) for B(2Alk)M hectorite. The value of < 500 mg/L for B(Alk)2M bentonite is presented because an EC₅₀ could not be determined from this study that used only one concentration. EC₅₀ values in other species (*Mysidopsis, Acartia tonsa*) for category members were similar or showed lower toxicity.
Data on acute toxicity to the aquatic plant *Skeletonema costatum* are available. The 72-hr $\text{ErC}_{50}$ (growth rate) was $>1,000 \text{ mg/L (nominal)}$ for 2M(2Alk) bentonite. In three tests using B(2Alk)M bentonite, the 72-hr $\text{ErC}_{50}$ values were 23.8, 82.3 and $>1,000 \text{ mg/L}$. It is likely that physical toxicity occurred in some studies, including the study reporting an $\text{Ec}_{50}$ of 23.8 mg/L; however, the study did not provide additional information regarding evidence of dispersed material. For B(2Alk)M hectorite, the 72-hr $\text{EbC}_{50}$, $\text{ErC}_{50}$ (0-24 hr), and NOEC were $>100$, $>100$, and 100 mg/L (nominal), respectively.

Chronic aquatic toxicity studies are also available for B(2Alk)M hectorite. A 21-day $\text{Ec}_{50}$ (reproduction) in *Daphnia magna* was 7.6 mg/L (nominal) and the NOEC was 3.2 mg/L. Mortalities (immobilization) that occurred at 32 mg/l were considered to be due in part to physical effects of the test material.

The LC$_{50}$s for 2M(2Alk) bentonite, 2M(2Alk) hectorite, and B(2Alk)M bentonite were $>10,000$, $>1,269$, and $>10,000$ mg/kg, respectively, when assessed for toxicity to a sediment re-worker mud shrimp (*Corophium volutator*).

Several terrestrial tests have also been conducted. In an earthworm acute toxicity test, the 14-d NOEC was 1,000 mg/kg for B(Alk)2M bentonite and B(2Alk)M hectorite. In a study of emergence and early growth stages of cress seedlings (*Lepidum sativum*) using B(2Alk)M hectorite, the LOEC was 1 mg/kg (no NOEC determined) and the LC$_{50}$ was 9 mg/kg. The $\text{Ec}_{50}$s were $>100$ mg/kg for the emergence and early growth stages of wheat and radish seedlings (*Tritium aestivum* and *Raphanus sativus*, respectively) exposed to B(2Alk)M hectorite. The NOECs were both 100 mg/kg, the highest doses tested.

**Exposure**

The 2005 production volumes for the USA (Sponsor country) were:

- B(Alk)2M hectorite = 1.46 million pounds (ca. 662 tonnes);
- 2M(2Alk) bentonite = 73.04 million pounds (ca. 33,130 tonnes);
- 2M(2Alk) hectorite = 9.31 million pounds (ca. 3223 tonnes);
- B(2Alk)M bentonite = 15.67 million pounds (ca. 7108 tonnes);
- B(2Alk)M montmorillonite = 0 million pounds (0 tonnes).

The common functional feature of the Organoclays Category is their use as rheological agents and/or additives for non-aqueous fluids. Rheological additives are materials that affect in a controlled and predictable way the flow properties of liquids or powders. Selection of the clay type, specific quaternary ammonium compound, and reaction conditions enables design of organoclays for specific applications.

The downstream uses of organoclay rheological additives, including approximate percentage, are:
- coatings including paints (43%);
- oil field applications including drilling muds (37%);
- printing inks (13%);
- cosmetics (3%); and, other, including remediation and nanocomposites (4%).

Closed systems are used in some facilities. In these facilities, the material is delivered in bags, dumped into a hopper with a capture exhaust. At other facilities, a portion of the processing may occur in open systems (e.g., loading of the material, discharging of final product, or the bagging station may be open), while other portions may be closed (e.g., drying and other processes). Some types of engineering controls are used in all manufacturing facilities. For example, depending on the facility, material loading will have a suction system; local area ventilation is used in areas not fully enclosed; dust collectors and simple ventilation are used and capture exhaust is employed. The product is stored in warehouses in sealed multi-wall craft paper bags, palletized, and heat-shrink-wrapped. The product leaves the manufacturing facility in sealed bags on trucks and is transferred to barges where the products are placed in shipping containers of various types. Generally, about 10-20 metric tons are sent by ship. On rare occasions (e.g. emergencies), less than one metric ton is shipped by airplane.
Worker exposure is most likely to occur during loading, discharging, bagging and sampling. There may also be minimal equipment leaks of fugitive dust. All routes of exposure (inhalation, dermal, and ingestion) are possible at the manufacturing level. However, the most likely exposure route is inhalation of dust, followed by dermal contact. At the bagging station, local area ventilation is used at all plants to ensure workers do not exceed 8 hour time-weighted exposure limits established by for example, ACGIH TLVs for Cristobalite silica, and Quartz silica; ACGIH TLV’s and OSHA PEL’s for Respirable Dust and Total Dust. Respirators are available for additional protection as needed. Dermal contact is minimized through the use of protective clothing. Industrial hygiene monitoring assessments for airborne contaminants have been conducted during manufacturing operations at two confidential locations. These assessments showed worker exposures that were less than the respective occupational exposure limits.

At the industrial customer level, use is predominantly in open systems, although some industrial customers’ systems are closed. For example, the 50-lb bags are opened at the customer site and dumped into a hopper. The hopper generally has suction, which draws the material into the process. Most customers use local area ventilation in areas that are not enclosed (for example, to minimize dust generation during bag emptying into mixing tanks). Exposures are most likely to occur at the bag dumping stations. As at the manufacturer, the industrial customer also typically employs a combination of local area ventilation and respirators at the majority of facilities to ensure workers do not exceed 8-hour time-weighted exposure limits for cristobalite and quartz silica as well as total and respirable dust established by ACGIH or OSHA.

Organoclay materials are used in industrial and personal consumer products such as solvent-borne paints and stains, in specialty coatings and adhesives, specialty sealants, cosmetics and personal care products (antiperspirants) and drilling fluids. When used in paints or adhesives, the organoclay material is encapsulated in the final product. Use of organoclays in cosmetics or personal care products may result in dermal and inhalation exposure. In paint, the average amount of organoclay in the final product is 0.5 to 0.7 %. Most other consumer products contain 1-3% or less of the total formulation. However, some products (e.g., for fireplace/stove home maintenance) may contain higher percentages (e.g., < 45% 2M(2Alk) bentonite in fireplace/stove repair paste and 1-10% 2M(2Alk) bentonite in plumbing putty). For oil drilling, most products contain 1-3% w/w of the total formulation. Less than 1% of organoclay powders as supplied will have particle sizes below 10 µm. For high quality consumer applications such as paints and coatings, inks, lubricating grease, cosmetic applications, etc., these materials are typically ground to an average particle size of ca. 75 µm. For organoclay agglomerates, principally used in oil based drilling fluids, particle sizes may range up to ca. 6 mm in diameter.

The quaternary ammonium compounds in the organoclays are tightly held to the clay by strong ionic forces and through chemiabsorption to the clay. In situations where the quaternary compounds are included in excess of the exchange capacity of the clay, that “excess” is likely to be chemiabsorbed to the clay and not fugitive. Under normal conditions of use it is very unlikely there would be exposure to the quaternary ammonium compounds themselves.

**Human Health:** The chemicals are currently of low priority for further work. The chemicals possess properties indicating a hazard for human health (minimal to moderate eye irritation, respiratory irritation observed in acute studies using high exposure levels, potential carcinogenicity from crystalline silica, which is an impurity in amounts up to 10 percent for some of the substances). Based on data presented in the sponsor country (relating to production in the Sponsor country which accounts for an unknown fraction of global production and relating to the use pattern in the Sponsor country), risk management measures are being applied in occupational settings (occupational limits for cristobalite silica and quartz silica and for respirable and total dust). Countries may desire to check their own risk management measures to determine whether there is a need for additional measures.

**Environment:** The chemicals are currently of low priority for further work due to their low hazard profile.