FINAL REPORT

Safety Assessment of Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate

ABSTRACT

Sodium Naphthalenesulfonate is described as a surfactant-hydrotope for use in cosmetic formulations, although there are currently no reported uses. Sodium Polynaphthalenesulfonate functions as an emulsion stabilizer, surfactant-hydrotope, and surfactant-suspending agent in many leave-on cosmetic formulations, including those used eye and facial makeup products. The manufacture of these ingredients begins with the reaction of naphthalene with sulfuric acid. The resulting naphthalenesulfonic acid is reacted with sodium hydroxide to form Sodium Naphthalenesulfonate, or with formaldehyde and water to form polynaphthalenesulfonic acid, which is further reacted with sodium hydroxide to form Sodium Polynaphthalenesulfonate. Only low residual formaldehyde concentrations are found. These compounds are not significantly toxic in acute and subchronic animal tests. Slight, transient irritation of the conjunctiva was seen with Sodium Polynaphthalenesulfonate powder. The polymeric form is suggested for use at concentrations between 0.1 and 0.4% in cosmetic formulations. Sodium Naphthalenesulfonate undiluted was a moderate eye irritant, but had minimal effects at 2% --- it is suggested for use in cosmetics at <2%. Sodium Naphthalenesulfonate was only mildly irritating when applied undiluted and was non irritating at 2% and 20%; no sensitization was seen in a maximization test. Neither compound absorbs light radiation in the regions of the spectrum that would suggest a possible photochemical toxicity. Both compounds were negative in bacterial mutagenesis test systems. Clinical tests of Sodium Naphthalenesulfonate at 0.2%, 1%, and 2% showed no irritation, cumulative irritation, or sensitization. The available data were not considered a sufficient basis to determine the safety of these ingredients as used in cosmetic formulations. The fundamental issue is skin absorption/penetration, and the potential toxicities that may exist if application of these ingredients to the skin or mucous membranes can lead to systemic exposure. The additional data needed include: (1) octanol/water partition coefficient; (2) dermal absorption; and (3) if there is significant dermal absorption or if significant quantities of the ingredients may contact mucous membranes or be ingested, then dermal reproductive and developmental toxicity data are needed; and if significantly absorbed, one genotoxicity assay in a mammalian system is needed; and if that study is positive then a 2 year dermal carcinogenesis study using NTP methods may be needed. Because there are additonal data needed in order to complete the safety assessment, the overall conclusion is that the available data are insufficient to support the safety of these ingredients for use in cosmetic products.

INTRODUCTION

The following is a compilation of studies concerning Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate. Most of the data are on Sodium Polynaphthalenesulfonate.

CHEMISTRY

Definition and Structure

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate (CAS No.

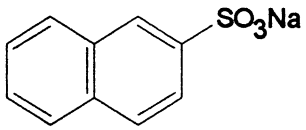
9084-06-4) is the sodium salt of the product obtained by the condensation polymerization of naphthalene sulfonic acid and formaldehyde. It has the following empirical formula (Wenninger and McEWen, 1997):

$$(C_{10}H_8O_3S \bullet CH_2O)_X \bullet xNa$$

Synonyms include Naphthalenesulfonic Acid, Polymer with Formaldehyde, Sodium Salt; and Sodium Salt of Sulfonated Naphthaleneformaldehyde Condensate (RTECS, 1997). In addition, the ingredient is known by numerous trade names such as: Atlox, Barra super, Bevaloid 35, Blancol dispersant, Darvan 1, Darvan No. 1, Daxad (11, 15, 18), Dispergator NF, Disperser NF, Dispersing agent NF, Dispersol ACA, Flube, Humifen NBL 85, Leukanol NF, Lissatan AC, Lomar (D, LS, PW), Na-Cemmix, NF, NF (dispersant), Pozzolith 400N, Surfactant NF, Tamol L, and Tamol SN (RTECS, 1997).

Sodium Naphthalenesulfonate

Sodium Naphthalenesulfonate (CAS No. 532-02-5) is the sodium salt of naphthalene sulfonic acid that conforms to the formula (Wenninger and McEwen, 1997):



Synonyms include: 2-naphthalenesulfonic acid, sodium salt; sodium beta-naphthalenesulfonate; and sodium 2-naphthalenesulfonate (RTECS, 1997).

Physical and Chemical Properties

The Table 1 is a summary of the physical and chemical properties of Sodium Polynaphthalenesulfonate also know as Tamol SN, Tamol L, and Daxad 11/15 (Rohm and Haas, 1994) (Hampshire Chemical Corp., 1995). The chemical and physical properties are listed in Table 2 (CTFA, 1999a).

TABLE 1
Chemical and Physical Properties of Sodium Polynapthalenesulfonate
(Hampshire Chemical Corp., 1995)

Property	Tamol SN	Tamol L	Daxad 11/15
Color	tan	brown	amber
State	powdered solid	liquid	powder
pH	8.8-10.0 (1% solution)	8.8-10.0	7-10.5 (1% solution)
Specific Gravity	0.4-0.7 bulk density	1.25	N.A.
Solubility in Water	completely soluble	dilutable	miscible
Percent Volatility	3-7% water	51-54% water	2-10% as water
Molecular Weight	N.A.	N.A.	3000-40000

TABLE 2
Chemical and Physical Properties of Sodium Napthalenesulfonate
(CTFA, 1999a)

Property	
Color	white to pale yellow
Density/Apparent	0.4
Solubility	soluble in water
pH at 25°C	5-7
Melting Point/Range	275°C

UV Absorption

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate absorbs UV light at a maximum of 225 nm ((Hampshire Chemical Corp., 1995).

Sodium Naphthalenesulfonate
FDA reports a maximum absorbance for Sodium Naphthalenesulfonate at 273 nm (FDA,1999).

Method Of Manufacture

Sodium Polynaphthalenesulfonate is made by reacting naphthalene with sulfuric acid under conditions of heat and pressure. Formaldehyde and water are then added to produce the acid polymer under the same conditions of heat and pressure. Caustic is added to the acid polymer resulting in the final product (Hampshire Chemical Corp., 1995).

Sodium Naphthalenesulfonate is made by reacting naphthalene with sulfuric acid. The resulting naphthalenesulfonic acid is then reacted with sodium hydroxide (Kao Corp., 1998).

Impurities

A supplier of Sodium Polynaphthalenesulfonate noted that one trade compound contained 41-44% Sodium Polynaphthalenesulfonate, 2-5% sodium sulfate, and 51-54% water. Another compound contained 86-88% Sodium Polynaphthalenesulfonate, 7-9% sodium sulfate, and 3-7% water. The two trade mixtures each contained 0.09% formaldehyde (max) (Rohm and Haas, 1994). (Note: In its safety assessment of Formaldehyde, the CIR Expert Panel concluded that a limit of 0.2% free formaldehyde was necessary to ensure safety (Elder, 1984).)

Limits for Sodium Polynaphthalenesulfonate suggested by one source are as follows: sulfate (as sodium sulfate) not more than 0.5%; heavy metals not more than 20 ppm; and, arsenic not more than 2 ppm ((Hampshire Chemical Corp., 1995).

One source listed the following limits for Sodium Naphthalenesulfonate: not more than 0.5% sulfate (as sodium sulfate); not more than 20 mg/kg of heavy metals; and, not more than 2 mg/kg arsenic. Formaldehyde is not used in the manufacture of Sodium Naphthalene-sulfonate (Kao Corp., 1998).

USE

Cosmetic

Sodium Polynaphthalenesulfonate is used in cosmetics as an emulsion stabilizer, surfactant - hydrotrope, and/or surfactant -suspending agent (Wenninger and McEWen, 1997). As of January 1998, there were 50 reported uses of Sodium Polynaphthalenesulfonate (FDA, 1998). See Table 1. Concentration of use data are no longer reported to the FDA (FDA, 1992). The Hampshire Corporations reported typical concentration of use to be between 0.1-0.4% (Hampshire Chemical Corp., 1995). Concentrations of use are shown in Table 4.

TABLE 3
Frequency of Use of Sodium Polynapthalenesulfonate
(FDA, 1998)

Product Category	No. Formulations in Category	No. Containing Ingredient
Eye Shadow	506	1
Mascara	167	8
Other Eye Makeup Preparations	120	3
Blushers (all types)	238	1
Foundations	287	6
Lipstick	790	1
Makeup Bases	132	25
Other Makeup Preparations	135	4
Moisturizing	769	1
1998 Total		**50**

TABLE 4
Concentration of Use Data of Sodium Polynapthalenesulfonate
(CTFA, 1999b)

Product Type	Reported Maximum Concentration
Mascara	0.3%
Other Eye Makeup Preparations	0.1%
Blushers (all types)	0.2%
Foundations	0.3%
Makeup Bases	0.3%

Sodium Naphthalenesulfonate is used in cosmetics as a surfactant -hydrotrope (Wenninger and McEwen, 1997). This ingredient was not reported in use in January 1998 (FDA, 1998). One source indicated that use was "typically below 2%" (Kao Corp., 1998).

ANIMAL TOXICOLOGY

Oral Toxicity

Acute

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate has an oral LD_{50} of 3.8 g/kg in rats (RTECS, 1997).

An azo-mixture containing 64.7% Sodium Polynaphthalenesulfonate had an oral LD_{50} of 0.37 g/kg in albino rats. A screening dose of 5.0 g/kg resulted in 90% mortality (MB Research Labs, 1981).

A 25% suspension of Sodium Polynaphthalenesulfonate (as Darvan No. 1) in water was administered intragastrically to albino rats. The oral LD_{50} was 3.25 g/kg (Food and Drug Research Labs, 1961).

Sodium Naphthalenesulfonate
Sodium Naphthalenesulfonate had an oral LD_{50} of 13.9 g/kg in rats (RTECS, 1997).

Subchronic

A trade compound containing 86% Sodium Polynaphthalenesulfonate was administered in feed at 0, 50, 150, 500, 1000, and 2500 ppm to groups of 10 male and 10 female rats for 90-days. There were no reported clinical signs of toxicity, feed consumption effects, or body weight effects. Also no changes in blood chemistry, blood counts, organ weights, or pathology were observed at any dose level. The NOEL for this study was reported at 500 ppm due to slight increases in urinary sugars in both males and females and urine protein concentrations in males (Rohm and Haas, 1998).

Dermal Toxicity

Acute

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate powder (as Darvan No. 1) (4, 8, 16 g/kg) was applied to the moistened depilated trunk of rabbits (1 inch of area was abraded). Two rabbits were tested at each dose. The material was wiped off after 24 h and rabbits observed for 14 days. Transient erythema and edema were observed. Using the Draize scale with a maximum score of 8, scores of 3 were noted in all rabbits on days 1 and 2. The reactions lessened during the two-week observation period; on day 14, rabbits dosed with 4 and 8 g/kg had zero scores and rabbits dosed with 16 g/kg had scores of 1. The approximate dermal LD_{50} > 16.0 g/kg (Food and Drug Research Labs, 1961).

Ocular Toxicity

Acute

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate powder (as Darvan No. 1) (10 mg) was instilled into one conjunctival sac of three rabbits. Eyes were scored according to the Draize scale (maximum score of 110). Slight, transient irritation of conjunctiva was observed; the cornea and iris were not affected. Individual scores were 14, 10, and 14 at the 4 h observation; 4, 4, 4 on day 1; 4, 4, 2 on day 2; and zero on days 4 and 7 (Food and Drug Research Labs, 1961).

Sodium Naphthalenesulfonate
Sodium Naphthalenesulfonate was in undiluted form a moderate eye irritant and a minimal eye irritant at 2% according to a OECD guideline 405 study (Hampshire Chemical Corp., 1995).

Dermal Irritation

Sodium Naphthalenesulfonate
Sodium Naphthalenesulfonate was tested according to the Draize method. A 24 h occlusive patch was applied to rabbits. It was a mild irritant when applied undiluted. It was a non-irritant at 2% and 20%. No additional details were provided (Kao Corp., 1998).

Dermal Sensitization

Sodium Naphthalenesulfonate
Sodium Naphthalenesulfonate was tested under the guinea pig maximization test (GPMT) and Buehler protocols. It did not sensitize any of the ten animals tested under each protocol. No additional details were provided (Kao Corp., 1998).

MUTAGENICITY

Sodium Polynaphthalenesulfonate
Sodium Polynaphthalenesulfonate (tan granules identified under the trade name Tamol SN) was tested in the Ames assay using *Salmonella typhimurium* strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538. It was negative both with and without metabolic activation at a dose range of 0.1-500 µg/plate (Litton Bionetics, Inc., 1977).

Sodium Naphthalenesulfonate
Sodium Naphthalenesulfonate was negative in an Ames assay using *Salmonella typhimurium* strains TA 98, TA 100, TA 1535, TA 1537, and TA 1538. No additional details were provided (Kao Corp., 1998).

CLINICAL ASSESSMENT OF SAFETY

Dermal Irritation and Sensitization

Sodium Naphthalenesulfonate
A 48 h occlusive patch containing 0.2% or 2% Sodium Naphthalenesulfonate was applied to 40 subjects. Reactions were similar to those observed with the water control. No additional details were provided (Kao Corp., 1998).

A 21-day cumulative irritation and sensitization study was conducted using 52 subjects. Occlusive patches containing 1% Sodium Naphthalenesulfonate were applied. The cumulative irritation index was 0.06 (scale not provided). No sensitization reaction was observed. No additional details were provided (Kao Corp., 1998).

SUMMARY

Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate are sodium salts of naphthalene sulfonic acid. Formaldehyde is used in the production of Sodium Polynaphthalenesulfonate and remains in the final product.

In January 1998, Sodium Polynaphthalenesulfonate was used in 50 formulations as an emulsion stabilizer, surfactant -hydrotrope, and/or surfactant -suspending agent. Sodium Naphthalenesulfonate functions as a surfactant - hydrotrope. The Kao Corporation reported Sodium Polynaphthalenesulfonate use at concentrations less than 2% (Kao Corp., 1998): one source reported that Sodium Polynaphthalenesulfonate is used at concentrations between 0.1-0.4% (Hampshire Chemical Corp., 1995).

Sodium Polynaphthalenesulfonate had an oral LD_{50} of 3.8 g/kg and Sodium Naphthalenesulfonate had an oral LD_{50} of 13.9 g/kg in rats. Sodium Polynaphthalenesulfonate had a dermal LD_{50} > 16.0 g/kg in rabbits.

The maximum absorbance for Sodium Polynaphthalenesulfonate was reported at 225 nm (Hampshire Chemical Corp., 1995); as for Sodium Naphthalenesulfonate, the FDA reported a maximum at 273 nm (FDA, 1999).

Both ingredients were negative in Ames assays.

In clinical studies, Sodium Naphthalenesulfonate was neither an irritant (tested up to 2%) nor a sensitizer (tested up to 1%).

DISCUSSION

Section 1, paragraph (p) of the CIR Procedures states that "A lack of information about an ingredient shall not be sufficient to justify a determination of safety." In accordance with Section 30(j)(2)(A) of the Procedures, the Expert Panel informed the public of its decision that the data on Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate were not sufficient for determination whether the ingredients, under relevant conditions of use, were either safe or unsafe. The Panel released a Notice of Insufficient Data on December 9, 1997 outlining the data needed to assess the safety of Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate. Comments received during the 90-day public comment period included acute oral toxicity, acute dermal toxicity, and ocular irritation. These submissions addressed the Panel's concerns regarding dermal and ocular

irritation. But additional concerns remain. Data needed to make a safety assessment are:

1. octanol/water partition coefficient;
2. dermal absorption;
3. if there is significant dermal absorption or if significant quantities of the ingredient may contact mucous membranes or be ingested, then dermal reproductive and developmental toxicity data are needed and if significantly absorbed, then one genotoxicity assay in a mammalian system is needed, and if that study is positive then a 2-year dermal carcinogenesis study using NTP methods may be needed .

CONCLUSION

The CIR Panel concludes that the available data are insufficient to support the safety of Sodium Polynaphthalenesulfonate and Sodium Naphthalenesulfonate for use in cosmetic products.

ACKNOWLEDGMENT

Bindu Nair, former Scientific Analyst & Writer, prepared this report assisted by Amy R. Elmore, Scientific Analyst and Writer.

REFERENCES

Ciba-Geigy Corp. (1977) Initial submission: skin irritation in the rabbit after single application of Fat 36091/A (containing Sodium Polynaphthalenesulfonate) with cover letter dated 100992. National Technical Information Service (NTIS) report No.: OTS0571844.

[1]CTFA. (1999a) CTFA chemical description of sodium napthalenesulfonate. (1 page) [1]

CTFA. (1999b) CTFA ingredient use data on sodium polynapthalenesulfonate. (1 page) [1]

Elder, RL. ed. (1984) Final Report on the Safety Assessment of Formaldehyde. *J Am Coll Toxicol.* 3(3):157-184.

FDA. (1998) Cosmetic product formulation data. *FDA database*. Washington, DC: FDA.

FDA. (1999) Spectra Library, Division of Cosmetics and Colors. *FDA database*. Washington, DC:FDA.

Food and Drug Research Laboratories. (1961). Screening tests of the oral, dermal, and mucous membrane toxicity of Darvan No. 1 (Sodium Polynaphthalenesulfonate). Unpublished data submitted by CTFA. (8 pages) [1]

Food and Drug Administration (FDA). (1992) Modification in Voluntary Filing of Cosmetic Product Ingredient and Cosmetic Raw Composition Statements. Final rule. *Federal Register* 57: 3128-30.

Hampshire Chemical Corporation. (1995) Concentration of use, method of manufacture, impurities and absorption data regarding Sodium Polynaphthalenesulfonate. Unpublished data submitted by CTFA. (7 pages) [1]

Industrial Bio-test Labs Inc. (1975) Initial submission: letter from Ciba-Geigy Corp to US EPA regarding acute toxicity studies with Cibanone Yellow GC paste (containing Sodium Polynaphthalenesulfonate) with attachments and cover letter dated 100992. NTIS report No.: OTS0571788.

Kao Corp. (1998) Concentration of use, method of manufacture, impurities, and results of an Ames assay, and dermal irritation and sensitization studies regarding Sodium Naphthalenesulfonate. Unpublished data submitted by CTFA. (2 pages) [1]

Litton Bionetics, Inc. (1977) Mutagenicity evaluation of TRC K82103 (containing Sodium Polynaphthalenesulfonate). Sponsored by Toms River Chemical and subsequently submitted to US EPA. in NTIS report No.: OTS0204489. (six microfiches. study found in microfiche #5, row 2. information concerning study on microfiches #1, and # 3, row 1.)

MB Research Laboratories. (1981) Initial submission: single dose oral toxicity in rats/acute oral LD_{50} in rats of Cibacete Orange 3RL granules (containing Sodium Polynaphthalenesulfonate) with cover letter dated 100992. NTIS report No.: OTS0571790.

Registry of Toxic Effects of Chemical Substances (RTECS). (1997) Sodium Polynaphthalenesulfonate and Sodium - Naphthalenesulfonate entries. *RTECS database*. Bethesda, MD: National Library of Medicine.

Rohm and Haas. (1994) Material safety data sheet and product info re: Tamol L conc and Tamol SN (dispersing agent) [Sodium Polynaphthalenesulfonate]. Unpublished data submitted by CTFA. (29 pages) [1]

Rohm and Haas. (1998) Subchronic oral toxicity study re: Tamol N (dispersing agent) [Sodium Polynaphthalenesulfonate]. Unpublished data submitted by CTFA. (1 page) [1]

Wenninger JA, McEwen GN Jr. eds. (1997) *International Cosmetic Ingredient Dictionary and Handbook*. 7th edn. Vol 2. Washington, D.C.: CTFA. p. 1293, 1302.

[1]Available for review: Director, Cosmetic Ingredient Review, 1101 7th Street, NW, Suite 310, Washington, DC 20036.