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**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION  
AND ASSESSMENT SCHEME**

**FULL PUBLIC REPORT**

**Amphoteric Polydimethylsiloxane**

This Assessment has been compiled in accordance with the provisions of *the Industrial Chemicals (Notification and Assessment) Act 1989, as amended* and Regulations. This legislation is an Act of the Commonwealth of Australia. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS) is administered by Worksafe Australia which also conducts the occupational health & safety assessment. The assessment of environmental hazard is conducted by the Department of the Environment, Sport, and Territories and the assessment of public health is conducted by the Department of Health, Housing, Local Government and Community Services.

For the purposes of subsection 78(1) of the Act, copies of this full public report may be inspected by the public at the Library, Worksafe Australia, 92-94 Parramatta Road, Camperdown NSW 2050, between the hours of 10.00 a.m. and 12.00 noon and 2.00 p.m. and 4.00 p.m. each week day except on public holidays.

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Director

Chemicals Notification and Assessment

**FULL PUBLIC REPORT****Amphoteric Polydimethylsiloxane****1. APPLICANT**

Salkat Australia Pty Ltd, 262 Highett Rd, Highett Vic 3190

**2. IDENTITY OF THE CHEMICAL**

Based on the nature of the chemical and the data provided, Amphoteric polydimethylsiloxane, is considered to be non-hazardous. Therefore, the chemical name, CAS No, molecular formula, structural formula, molecular weight, monomer composition and spectral data have been exempted from publication in the Full Public Report and the Summary Report.

**Trade name:** ABIL B 9950 (30% polymer solution)

**Other names:** Amphoteric polydimethylsiloxane (polymer); Polysiloxane betaine (30% polymer solution)

**Maximum percentage of low molecular weight species**

**(molecular weight < 1000):** <18%, based on GPC of a polymer intermediate, Siloxanes and silicones, dimethyl, methyl 3-(oxiranyl-methoxypropyl) Prepolymer I

**Method of detection and determination:** NMR spectrometry; gas chromatography.

**3. PHYSICAL AND CHEMICAL PROPERTIES**

The notified polymer will be imported as a 30% solution in 1,2-propanediol/sodium chloride/water. The following physico-chemical properties relate to the imported solution.

<b>Appearance at 20°C and 101.3 kPa:</b>	viscous amber liquid
<b>Odour:</b>	faint, not described
<b>Specific Gravity:</b>	1070 kg/m <sup>3</sup> @ 25°C
<b>Water Solubility:</b>	expected to be completely soluble at all ratios (>80g/L), however, at high concentrations a homogeneous mixture could only be reached after 24 h
<b>Viscosity:</b>	~60 mPa.S @ 25°C
<b>pH:</b>	~6 (40g/L in water @ 20°C)
<b>Flash Point:</b>	>100°C
<b>Particle size distribution:</b>	not applicable as the chemical is a liquid
<b>Hydrolysis as a function of pH:</b>	the notifier states that no hydrolysis is expected @ pH 4 - 9 (cleavage of Si-O-Si bonds will occur @ pH <2 or >11 at temperatures >90°C)
<b>Adsorption/desorption:</b>	not measured
<b>Thermal stability:</b>	cleavage of Si-O-Si bonds will occur at temperatures > 90°C
<b>Dissociation Constant:</b>	expected to dissociate completely
<b>Explosive Properties:</b>	no details given
<b>Reactivity/Stability:</b>	no details given
<b>Comments on missing data:</b>	

Vapour Pressure was not measured. Due to the polymeric nature and the fact that the new chemical substance is a salt a significant vapour pressure is not expected.

No values were provided for melting point/boiling point. As the chemical is highly viscous, methods of measuring/estimating melting and boiling points are not applicable.

#### **Notes on physico-chemical properties:**

The environmental properties of polydimethylsiloxane fluids have been well reviewed by Hamelink (1).

Silicone fluids are very surface active because the flexible siloxane linkages permit alignment of the hydrophobic methyl substituents towards the non-polar phase, and of the polysiloxane backbone towards the polar phase. This particular silicone has increased hydrophilicity because of the amphoteric substituents.

The polar medium is generally water, and apolar media to which polydimethylsiloxanes become attached may be textiles, sewage sludge, algae, sediment etc. In aqueous environments, strong, complete and permanent adsorption of high molecular weight silicone fluids to sediment may be assumed.

Data such as solubility and partition coefficient are not particularly relevant to surface active compounds, which prefer to reside at or on the interface between polar and apolar media, rather than partitioning between them. Polydimethylsiloxanes are generally extremely hydrophobic, but according to the submission, modification as in the present case favours solubilisation via formation of water dispersed structurally ordered aggregates.

The extent to which hydrolysis would occur in the environment is unclear, given that silicones adsorb strongly to surfaces. However, the hydrophilic substituents can be expected to project into the aqueous phase where they may be available for microbial attack.

#### **4. PURITY OF THE CHEMICAL**

The following impurity proportions are based on 18% low molecular weight species as determined by GPC of a polymer intermediate. The volatile impurities were determined by GC of the notified polymer. Estimate values were provided for residual reactants, however, these have been exempted from publication in the Full Public Report and the Summary Report as they are present at

levels below the cut-off concentration for classifying the notified polymer as a hazardous substance (2).

**Degree of purity:** 82%

**Toxic or hazardous impurities:**

(a) **Chemical name:** 1,2-propanediol  
**Synonyms:** 1,2-dihydroxypropane; methyl glycol; propylene glycol; trimethyl glycol  
**CAS No.:** 57-55-6  
**Weight percentage:** 0.25  
**Toxic properties:** human eye and skin irritant; oral rat LD50 20 g/kg; slightly toxic by ingestion skin contact intraperitoneal, intravenous, subcutaneous and intramuscular routes; experimental teratogenic and reproductive effects; mutagenic data (3)

**Non-hazardous impurities:** 14.8% (total)

**Unidentified impurities:** 3% (partially identified as disiloxane, hexasiloxane, pentasiloxane, silanol, propanol, toluene)

**Maximum content of residual monomers/reactants:** <0.4%

**Additives/Adjuvants:**

<b>Chemical Name:</b>	<b>CAS No.:</b>	<b>Weight percentage:</b>
1,2-propanediol	57-55-6	40
Sodium chloride	7647-14-5	3.5
Water		26.5

**5. INDUSTRIAL USE**

The notified polymer will be imported as a 30% solution in 1,2-propanediol/sodium chloride/water, to be used as an ingredient/additive in cosmetic formulations. Initially the polymer will be used at one site in the manufacture of Nivea Foaming Face Wash. For this application it is estimated that 60 kg of polymer will be imported in the first year increasing to 150 kg by the fifth year.

## **6. OCCUPATIONAL EXPOSURE**

The notified polymer will be imported in 50 kg drums as a 30% solution in 1,2-propanediol/sodium chloride/water. It will be transported by road to Smith & Nephew Pty Ltd, Clayton, Vic. Workers at this site will weigh and mix the polymer solution into the cosmetic formulation, Nivea Foaming Face Wash, and package the final product for distribution to supermarkets and pharmacies. ABIL B 9950 will constitute 1.2% of the face wash. Therefore, the notified polymer will make up 0.4% of the face wash.

At Smith & Nephew, approximately 16 workers will be potentially exposed to the notified chemical. One batch of 500 kg of product is anticipated to be manufactured every fortnight. One worker will weigh out the required amount of ABIL B 9950 and other ingredients, add these to a mixing tank, and clean out the mixing and holding tanks after completion of each batch (involving exposure for approximately half hour/batch to the undiluted ABIL B 9950 solution and 5 hours/batch to the mix); 4 workers will check the weights and prime the pump equipment used for filling and packing (approximate exposure: 5 hours/batch to the incorporated polymer); one worker will maintain and and clean the filling equipment (approximate exposure: 4 hours/batch to the incorporated polymer); 2 quality control personnel will make in-process routine checks of weights and product (approximate exposure: half an hour/batch); and 8 workers will move and store raw and finished product (approximate exposure: 2 hours/batch).

## **7. PUBLIC EXPOSURE**

The notified polymer will be used in the manufacture of Nivea Foaming Face Wash. The face wash, containing an estimated 0.4% w/w of the notified polymer, will be sold to the public through supermarkets and pharmacies.

## **8. ENVIRONMENTAL EXPOSURE**

### **. Release**

The extent of environmental release arising from formulation is unclear as details of the process were not made available.

## . **Fate**

The notified substance is amphiphilic in nature, i.e. it has both hydrophobic and hydrophilic substituents. However, the length of the hydrophobic backbone and the relatively low number of hydrophilic substituents suggest that this modified silicone will be removed from solution by adsorption onto sludge with little, if any, likely to be contained in treated waste waters. Sludge containing the notified substance may then be incinerated or landfilled. Incineration would destroy the substance and liberate oxides of carbon, nitrogen and silicon, while disposal to landfill would immobilise it.

Polydimethylsiloxanes are thought to be unstable in terrestrial environments, where clays can catalyse cleavage of the siloxane linkage, but are probably more permanent in aquatic sediment as the catalytic action of clays is inversely related to their degree of hydration (3).

As noted above, the hydrolytic stability of this modified silicone is unclear. However, hydrolysis products do not appear to be of significant ecological concern.

## 9. **EVALUATION OF TOXICOLOGICAL DATA**

Toxicological data were submitted for ABIL B 9950 (30% polymer solution) although not required for polymers of number-average molecular weight (NAMW) > 1000 under the *Industrial Chemicals (Notification and Assessment) Act 1989, as amended* (the Act). These data are evaluated below.

### 9.1 **Acute Toxicity**

Table 1 Summary of the acute toxicity of ABIL B 9950 (30% polymer solution)

Test	Species	Outcome	Reference
Oral	Rat	LD50 >5000 mg/kg	4
Skin	Rabbit	non-irritant	5
Eye	Rabbit	slight irritant	6

#### **9.1.1 Oral Toxicity (4)**

This study was conducted in accordance with OECD guideline : 401 (7).

ABIL B 9950 was administered to 10 Sprague-Dawley rats (5 male and 5 female) by oral gavage, at a single dose of 5000 mg/kg. Clinical observations were made over a 14-day period. No deaths occurred during the observation period. All rats were sacrificed on day 14. Necropsy was not performed. Bodyweight gain of the treated animals was unaffected and no clinical signs were noted.

Results of this study indicate an acute oral LD<sub>50</sub> of >5000 mg/kg in rats of both sexes for ABIL B 9950.

#### **9.1.2 Skin Irritation (5)**

A single dose of 0.5 ml ABIL B 9950 was applied by semi-occlusive application to the closely-clipped dorsa of 6 New Zealand white rabbits (1 male and 2 females); 1 abraded and 1 intact site per animal. Twenty-four hours later the dressings were removed and the test site wiped clean. Skin reactions were assessed immediately and 48 hours after dressing removal. No clinical symptoms or mortality were observed in the animals during the study. Slight to well-defined erythema was observed at all abraded and 3 intact sites immediately after dressing removal. No skin effects were apparent 48 hours later. No edema or corrosive effects were observed on the skin of any animals during the study.

Results of this study indicate that ABIL B 9950 is not a skin irritant in rabbits.

#### **9.1.3 Eye Irritation (6)**

This study was conducted in accordance with OECD guideline No: 405 (8).

A single dose of 0.1 ml ABIL B 9950 was instilled in the conjunctival sac of the left right eye of each of 6 New Zealand white rabbits. The left eye served as the control. The eyes were examined 24, 48 and 72 hours after treatment. Slight conjunctival irritation was observed at 24 hours for each animal.



By 48 hours half of the treated eyes had cleared, and by 72 all had cleared. No corneal opacity or iridial damage was observed. No deaths occurred and no clinical symptoms were observed during the study.

The results of this study suggest that ABIL B 9950 is a slight eye irritant in rabbits.

### **9.3 Overall Assessment of Toxicological Data**

Animal tests suggest that ABIL B 9950 has low acute oral toxicity (rat LD<sub>50</sub> >5000 mg/kg), is not a skin irritant but is a slight eye irritant.

## **10. ASSESSMENT OF ENVIRONMENTAL EFFECTS**

No ecotoxicological data were provided, which is acceptable for polymers of NAMW > 1000 according to the Act. The high molecular weight of the substance suggests that it will not cross biological membranes, and will therefore be of low toxicity. It is well accepted that polydimethylsiloxane fluids become permanent residents of sediment but should not exert adverse environmental effects. Physical effects such as surface entrapment have been observed when testing aquatic invertebrates in clean laboratory water, but similar effects are not expected in natural environments where a large variety of other surfaces provide opportunities for deposition (3).

While the polymer contains quaternary ammonium functionalities, which are known to interact with gill membranes, environmental behaviour of this modified silicone is expected to be dominated by the siloxane backbone, which will align itself at or on surfaces.

The toxicity of quaternary ammonium compounds is known to be greatly reduced in the environment because of preferential binding to dissolved organics in surface water (9), and the hydrophobic properties of the polydimethylsiloxane chain will further moderate any toxic potential.

## **11. ASSESSMENT OF ENVIRONMENTAL HAZARD**

As noted above, the notifier has been unable to provide estimates of typical amounts and concentrations of this modified silicone

likely to be discharged from the formulation plant. However, the notifier has confirmed that a maximum of 500 kg of ABIL B 9950 will be used exclusively in the manufacture of the product, Nivea Foaming Face Wash, in quantities of 1.2% w/w. Given that the raw chemical is imported as a 30% solution in a water/1, 2-propanediol mixture (7:4), the maximum amount of raw chemical imported is 150 kg.

If the polymer remains solubilised, a predicted environmental concentration (PEC) for the substance in sewage water throughout Australia can be estimated from the following assumptions:

- 150 kg maximum annual use amongst an Australian population of 17 million; and
- a daily per capita water usage volume of 150 L (i.e. national usage = 930.8 GL per annum).

This provides a PEC of 0.16 ppb in sewage water which would be further reduced to minute levels, in the range of parts per trillion (ppt), by precipitation or dilution in receiving waters. Therefore, the above exercise confirms that unacceptable concentrations of the new modified silicone fluid should not enter the environment.

Water soluble, polyether substituted polydimethylsiloxane fluids are widely used as toiletry products, applications which involve potential aquatic exposure.

The introduction of a similar compound for cosmetic use is not expected to lead to a significant increase in environmental hazard, given the biocompatible nature of these substances.

## **12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS**

The notified polymer has a NAMW > 1000 and is therefore unlikely to cross biological membranes and cause significant systemic effects. The polymer contains up to 18% (w/w) low molecular weight (<1000) species, of which <0.6% are identified as hazardous (0.25% 1,2-propanediol; <0.301% residual monomers/reactants).

ABIL B 9950 (30% polymer solution) has been shown in animal studies to have low acute toxicity, be non-irritating to the skin

and slightly irritating to the eyes. The irritant effects in the eye may be due to the solvent 1,2-propanediol, which is a known human skin and eye irritant.

Under normal use conditions, with appropriate control measures and/or precautions to minimise contact, the notified polymer is not expected to present any significant health or safety hazard to workers.

There is a high potential for public exposure to the notified chemical since it is to be sold to the public for use as a face wash. However, the concentration of the notified polymer in the cosmetic product is only 0.4%, and due to the high molecular weight of the notified polymer it is considered that absorption through biological membranes would be minimal. As a result there should be negligible risk to public safety.

### **13. RECOMMENDATIONS**

To minimise occupational exposure to Amphoteric polydimethylsiloxane the following guidelines and precautions should be observed:

- . If engineering controls are insufficient to reduce exposure to a safe level during product manufacture, the following personal protection equipment should be worn:
  - . goggles, or full face shield where splashing is possible, conforming to AS 1336 (10) and AS 1337 (11);
  - . impervious gloves conforming to AS 2161 (12); and
  - . protective clothing conforming to AS 3765.1 (13) or AS 3765.2 (14).
- . Good work practices should be implemented to avoid spillages or splashings.
- . Good personal hygiene practices, such as washing of hands prior to eating food, should be observed.
- . A copy of the Material Safety Data sheet for the new chemical or products containing it should be easily accessible to workers.

#### **14. MATERIAL SAFETY DATA SHEET**

The Material Safety Data Sheet (MSDS) for ABIL B 9950 (Attachment 1) was provided in Worksafe Australia format (15). This MSDS was provided by Salkat Australia Pty Ltd as part of their notification statement. It is reproduced here as a matter of public record. The accuracy of this information remains the responsibility of Salkat Australia Pty Ltd.

#### **15. REQUIREMENTS FOR SECONDARY NOTIFICATION**

Under the *Industrial Chemicals (Notification and Assessment) Act 1989, as amended* (the Act), secondary notification of Amphoteric polydimethylsiloxane shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

#### **16. REFERENCES**

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7. OECD Guidelines for Testing of chemicals - *Acute Oral Toxicity* No: 401, 1981.

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