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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

Calcium xylene sulphonate

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT

Calcium xylene sulphonate

1. APPLICANT

Proctor and Gamble Australia Pty Ltd of 99 Phillip Street PARRAMATTA NSW 2150 has submitted a standard notification statement in support of their application for an assessment certificate for calcium xylene sulphonate.

2. IDENTITY OF THE CHEMICAL

The notifier has not claimed any information to be exempt from publication in Full Public and Summary Reports.

Chemical Name: calcium xylene sulphonate

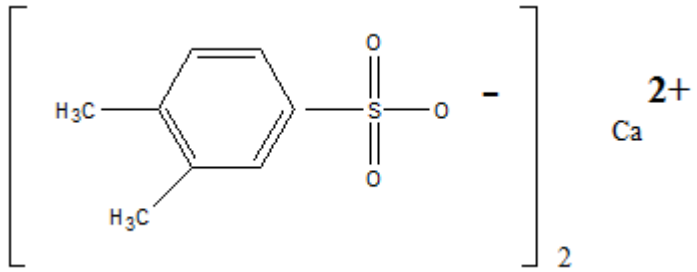
Chemical Abstracts Service (CAS) Registry No.: 28088-63-3

Other Names: dimethylbenzene sulphonic acid, calcium salt

Marketing Name: Naxonate CSX

Molecular Formula: $(C_8H_9SO_3)_2Ca$

Structural Formula:



Molecular Weight: 410

Method of Detection and Determination: UV/Visible spectroscopy

Comments on Chemical Identity

The new compound is the calcium salt of xylene sulphonic acid, and is very soluble in water, capable of forming solutions containing up to 35% of the new compound - see physico-chemical properties below.

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	clear liquid
Boiling Point:	100°C
Specific Gravity:	1.3 $\pm$ 0.0052
Vapour Pressure:	not provided (see comments below)
Water Solubility:	553$\pm$4 g/L at 20°C
Partition Co-efficient (n-octanol/water):	log K_{ow} =2.70$\pm$0.01 at 21$\pm$1°C
Hydrolysis as a Function of pH:	not provided (see comments below)
Adsorption/Desorption:	not provided (see comments below)
Dissociation Constant:	not provided (see comments below)
Flash Point:	not applicable
Flammability Limits:	none
Autoignition Temperature:	not provided
Explosive Properties:	not provided
Reactivity/Stability:	may react with oxidising agents

Comments on Physico-Chemical Properties

The notifier did not supply vapour pressure data for the new chemical, but the ionic salt nature of the material indicates that this would be very low.

Water solubility was determined using the flask method. In this procedure saturated solutions are prepared by stirring an excess of the compound with a known volume of water for periods of 24, 48 and 72 hours in a water bath at 30ºC. After these periods each solution was allowed to equilibrate at 20ºC for 24 hours, and the concentration of the test material in the aqueous phase determined (after suitable dilution) using High Performance Liquid

Chromatography (HPLC). Each test was performed in duplicate, and at 20ºC the mean concentration in the solution prepared after 24 hours stirring was 549±2 g/L, while that in the solution prepared after 72 hours was 557±1 g/L. These very similar values indicate that they reflect the true water solubility of the material, and the mean of all six separate determinations gave a water solubility of 553±4 g/L at 20ºC.

No data on hydrolytic degradation was supplied with the notification, but the compound contains no bonds which are susceptible to hydrolysis under the environmental pH region where 4<pH<9, and so it is expected to be stable.

The n-octanol/water partition coefficient was determined using the flask method where an aqueous solution initially containing 953 g/L of the new compound was shaken with n-octanol over a 24 hour period at a temperature maintained at 21±1ºC. The organic and aqueous phases were separated through centrifugation, and each analysed for the chemical using HPLC. The partition coefficient Kow was determined as the ratio of concentration in n-octanol to that in the aqueous phase. This ratio was determined as 0.002± 0.00004, giving Log P_{ow} as –2.70±0.01. A low value for Log P_{ow} is expected for ionic material such as the new compound.

Adsorption/desorption data was not presented in the submission, but the very high water solubility and low value of partition coefficient indicates the new compound would not associate with soils and sediments.

No dissociation constant data was submitted with the notification, but the new compound is the calcium salt of a strong acid xylene sulphonic acid. The pK_a of this moiety is around 2.3, so the compound is expected to remain ionised in the environmental pH range.

4. PURITY OF THE CHEMICAL

Degree of Purity: 99%

Hazardous Impurities:

Chemical name:	dimethylbenzene
Synonyms:	xylene
CAS No.:	1330-20-7
Weight percentage:	< 1%
Regulatory Controls	national exposure standard 80 ppm TWA, 150 ppm STEL (NOHSC, 1995)
Toxic properties:	R20/21 Harmful by inhalation and in contact with skin R38 Irritating to skin (NOHSC, 1999a)

Non-hazardous Impurities (> 1% by weight): none

Additives/Adjuvants:

Chemical name:	sodium xylene sulphonate
CAS No.:	1300-72-7
Weight percentage:	5-15%
Chemical name:	water
CAS No.:	7732-18-5
Weight percentage:	60-70%

5. USE, VOLUME AND FORMULATION

The notified chemical is a component at 25-30% in the product Naxonate CSX stabilizer, which contains the additives tabulated above. This product will not be introduced to Australia, and the notified chemical will be introduced at a concentration of 3.41% in a finished dishwashing liquid, which will be marketed as Dawn.

The expected import volume is 66 tonnes per annum for the next five years.

6. OCCUPATIONAL EXPOSURE

The notified chemical will be imported as a component of a finished dishwashing liquid. It will be imported in 434 mL moulded plastic bottles for retail sale. No reformulation or re-packaging will be carried out.

Transport and Storage
The bottles containing the notified chemical will be imported in cardboard cartons, each containing 12 bottles. The cartons will be packed in containers. The containers will be transferred by road transport to a bunded area in the notifier's warehouse, from where these will be distributed to retail outlets including supermarkets and convenience stores. The notifier indicates that waterside, transport and warehouse workers will wear coats and heavy duty gloves. No worker exposure is expected during these operations except in case of an accident causing damage to the packaging. Dermal and ocular exposure may occur only in the event of a leak or spill. Inhalation exposure is not expected to occur due to very low vapor pressure of the notified chemical.

The notifier estimates that 50 waterside and transport workers will handle the packaged product containing the notified chemical, 12 times per year for 8 hours per day. Also up to 30 warehouse workers will handle the product containing the notified chemical, 100 times per year for 4 hours per day.

Retail
A large number of retail workers will be involved in handling the packaged product containing the notified chemical, in supermarkets, pharmacies and department/variety stores. The workers would generally handle the plastic bottles while opening cartons and stacking

shelves, and while processing purchases. Worker exposure could only occur in the event of a spill, when clean-up is required.

The notifier estimates that approximately 10 000 workers will handle the notified chemical, 100 times per year, for 1 hour per day.

Wash-up workers in commercial premises may use and be exposed to the notified chemical.

7. PUBLIC EXPOSURE

Public exposure to the notified chemical is expected to be widespread as the product containing the notified chemical will be sold to the public and used as washing-up liquid. Exposure will primarily occur via the dermal route, with the possibility of accidental ocular and oral exposure. The notified chemical is present at a concentration of 3.41% in the end-use product, which will normally be used diluted further prior to use. Public exposure during transport and storage is expected to be negligible.

8. ENVIRONMENTAL EXPOSURE

Release

The use pattern of the dishwashing liquid is such that almost all of the new compound will be released to the sewer system. Very little of the dishwashing concentrate is likely to be left in the bottles, since these are usually washed out with water prior to disposal. Any residual left in the bottles (ie not washed out) would be disposed of to landfill with general domestic waste.

Once released to the sewer system, the high water solubility and low Log P_{ow} indicates that the chemical would have little affinity for sludges and sediments. If released to these media the new compound is expected to be very mobile, and would enter the aquatic compartment.

Fate

Almost all of the new chemical is expected to be released to the water compartment through the sewer system, and remain in the water column. The chemical is expected to be stable to hydrolytic degradation. Consequently, the major routes for degradation and elimination of the compound in the environment are expected to be primarily biological (bacteriological) processes.

Biodegradation

The notifier has indicated that the new compound is biodegradable, and in the notification provided test reports for a Modified Sturm Test and a Semi Continuous Activated Sludge (SCAS) Test.

The carbon dioxide (CO_2) evolution test was performed in nutrient media inoculated with sewage microorganisms obtained from a sewage treatment plant. The level of dissolved organic carbon (DOC), together with the amount of carbon dioxide evolution was monitored

over a 29 day test period. The test vessels were maintained at room temperature, ie at temperatures between 20 and 25ºC. One test was conducted with test material added to give 10 mg/L of added organic carbon, and the second with 20 mg/L. A reference test was also run containing dextrose, together with a blank containing no added test or reference material.

The degree of biodegradation after 28 days, estimated through analysis for DOC for the media originally containing the new chemical at 10 mg/L was 85.6% and at 20 mg/L was 75.2%. The reference material had been degraded 85.6% under the same conditions. The degree of degradation as estimated from the evolution of CO_2 was 86% for the 10 mg/L test, 89% for the 20 mg/L test and 112.9% for the dextrose reference. The latter degree of degradation indicates that the bacterial culture was viable.

The results of these tests indicate that the new chemical is biodegradable under aerobic conditions. However, the CO_2 evolution curves included in the test report indicated that 10% degradation was achieved after approximately 3-4 days, but that after 14 days the degree of degradation was between 50 and 60%. Accordingly, while the results indicate that the compound is inherently biodegradable, the material may not be classified as being readily biodegradable according to the protocols of OECD TG 301 B. It should also be noted that the reference compound dextrose was degraded to more than 60% after the first six days of the test.

The Modified SCAS test was conducted in accordance with the protocols of OECD TG 302 A in order to simulate degradation of the compound in the aerated chambers of a sewage treatment plant. The test was conducted by introducing the test compound (at a nominal concentration equivalent to around 20 mg/L of organic carbon) with synthetic sewage (prepared from glucose, beef extract, nutrients and inorganic salts) at a constant rate into an aerated vessel containing activated sludge. The sludge had been previously acclimatised to the synthetic sewage feed and the test substance for a period of 14 days, namely 7 days with synthetic sewage only, followed by a second 7 days in which levels of the test material were gradually raised to the equivalent of 20 mg/L of organic carbon. The test was run in duplicate with an additional two control SCAS units to which artificial sewage alone was fed.

The temperature of all SCAS units was maintained at 20±2ºC, and the Total Organic Carbon (TOC) content of both the feed and effluent from the SCAS units were monitored periodically throughout the 7 day test period. The degree of removal of TOC from the control units was consistently high, typically 93.5%. These rates were compared (on a daily basis) to those for the SCAS units also fed with the test material, and the differences used to calculate the degree of degradation of the test substance assumed present in the feed at a level equivalent to 20 mg/L of dissolved carbon. The outcome of these test was that the new material was degraded to 94.7± 2.7%.

Bioaccumulation

The highly soluble nature of the compound indicates that it is not likely to have significant potential for bioaccumulation.

9. EVALUATION OF TOXICOLOGICAL DATA

A subchronic 91-day oral feeding study in rats was conducted using the analogue sodium xylene sulphonate (sodium salt of the notified chemical) and skin sensitisation study conducted using S10737.01 which is a formulation (light duty liquid) containing the notified chemical at 3.6%. Acute dermal toxicity, eye and skin irritation studies were conducted using 31.2% of the notified chemical.

9.1 Acute Toxicity

Summary of the acute toxicity of calcium xylene sulfonate

Test	*Species*	*Outcome*	*Reference*
acute oral toxicity	Rat	LD_{50} = 3 346 mg/kg	(Page, 1994a)
acute dermal toxicity	Rabbit	LD_{50}>2 000 mg/kg	(Page, 1994b)
skin irritation	Rabbit	Non-irritating	(Page, 1994c)
eye irritation	Rabbit	Mildly irritating	(Page, 1994d)
skin sensitisation	Guinea pig	Non-sensitising (analogue data)	(Merriman, 1997)

9.1.1 Oral Toxicity (Page, 1994a)

Species/strain:	Rat/Crl:CD
Number/sex of animals:	5/sex/group
Observation period:	15 days
Method of administration:	Oral gavage; 2 500, 3 000 3 300, 3 500, 4 000 and 5 000 mg/kg as a solution in deionised water at a constant volume of 20 mL/kg.
Test method:	US EPA 40 CFR Part 798
Mortality:	Mortality was observed at dosages of 3 000 mg/kg and greater during the 4-hour post-dose observation interval on study day 1, and on study day 2. All animals at 4000 and 5000 mg/kg died. No mortality was observed at 2500 mg/kg.
Clinical observations:	The predominant observations were decreased activity, anogenital staining, ptosis and prostration. Except for anogenital staining, the observations were primarily noted 1-4 hours after administration. Anogenital staining was noted on or between study day 2 and study day 5.
Morphological findings:	The predominant post-mortem observation was a trace to

	moderate red diffuse discolouration of the mucosa of the glandular stomach in animals that died during the study.
Comment:	No remarkable changes in body weights of the surviving animals were observed.
LD_{50}:	3 346 mg/kg
Result:	The notified chemical was of very low acute oral toxicity in rats.

9.1.2 Dermal Toxicity (Page, 1994b)

Species/strain:	Rabbit/New Zealand White
Number/sex of animals:	5/sex
Observation period:	15 days
Method of administration:	A single semi occluded application of 31.2% solution of the test substance at 2 000 mg/kg was applied to the shaven, intact skin.
Test method:	US EPA 40 CFR Part 798, Section 798.11
Mortality:	All animals survived to study termination.
Clinical observations:	Four of the ten animals displayed no visible abnormalities throughout the study. Erythema was noted on study day 3 in six animals with desquamation additionally observed in study day 9 in one animal. Except for two animals, these findings were observed through the remainder of the study.
Morphological findings:	At the post-mortem examination, no visible abnormalities were observed in six animals. The remaining four animals displayed focal or multifocal red discolouration of the treated skin with one animal additionally displaying desquamation of the same site. For one animal, the macroscopic observation did not agree with the clinical observation.
Comment:	Although no animal displayed a remarkable body weight change during week 1, body weight loss was noted in eight animals during study week 2.
LD_{50}:	> 2 000 mg/kg
Result:	The notified chemical was of low dermal toxicity in rabbits.

9.1.3 Inhalation Toxicity

The notifier stated that no inhalation study was performed, as the notified chemical is an aqueous solution with a vapour pressure similar to water.

9.1.4 Skin Irritation (Page, 1994c)

Species/strain:	Rabbit/New Zealand White
Number/sex of animals:	3/sex
Observation period:	3 days
Method of administration:	A volume of 0.5 mL containing 31.2% of test substance was applied under a 1-inch square gauze patch and secured with tape for 4 hours to a prepared site on the back of each animal.
Test method:	US EPA 40 CFR Part 798
Comment:	The test sites were evaluated at approximately 50 minutes and at 24, 48 and 72 hours after patch removal. No dermal irritation was observed in any animal during the study period. No tabulated data were presented by the testing laboratory. All animals survived to study termination.
Result:	The notified chemical was non-irritating to the skin of rabbits.

9.1.5 Eye Irritation (Page, 1994d)

Species/strain:	Rabbit/New Zealand White
Number/sex of animals:	3/sex
Observation period:	3 days
Method of administration:	0.1 mL of 31.2% undiluted test substance was instilled into the conjunctival sac of the right eye of each animal and the lids were held shut for about 1 second and released. The left eye served as control.
Test method:	US EPA 40 CFR Part 798, Section 798.4500

Draize scores (Draize, 1959) of unirrigated eyes:

	Time after instillation											
Animal	***1 hour***			***1 day***			***2 days***			***3 days***		
Cornea	***o***		***a***	***o***		***a***	***o***		***a***	***o***		***a***
1	[1]0		0	0		0	0		0	0		0
2	0		0	0		0	0		0	0		0
3	0		0	0		0	0		0	0		0
4F	0		0	0		0	0		0	0		0
5F	0		0	0		0	0		0	0		0
Iris												
1		1			0			0			0	
2		1			0			0			0	
3		1			0			0			0	
4F		1			1			0			0	
5F		1			0			0			0	
Conjunctiva	***r***	***c***	***d***	***r***	***c***	***d***	***r***	***c***	***d***	***r***	***c***	***d***
1	3	2	2	2	1	0	0	0	0	0	0	0
2	3	2	2	1	1	0	0	0	0	0	0	0
3	3	2	2	2	1	0	1	0	0	0	0	0
4	3	3	2	2	1	0	1	0	0	0	0	0
5	2	2	1	1	1	0	0	0	0	0	0	0

[1] see Attachment 1 for Draize scales F = female
o = opacity a = area r = redness c = chemosis d = discharge

Comment:

Animal 6 was excluded form the study because the test eye was determined to have a congenital abnormality.

<u>Group mean scores (24, 48 and 72 hour observation):</u>
Corneal opacity: 0
Irideal lesions: 0.067
Conjunctival redness: 0.67
Conjunctival chemosis: 0.33

Occular irritation to the five remaining animals was limited to the iris and conjunctiva. Peak irritation was observed 1 hour post-instillation but all lesions had resolved by 72 hours.

All rabbits survived to study termination.

Result:

The notified chemical was mildly irritating to the eyes of

rabbits.

9.1.6 Skin Sensitisation with an analogue substance, S10737.01, using the modified Buehler method (Merriman, 1997)

Species/strain:	Guinea pig/Hartley-derived
Number of animals:	5/sex
Induction procedure:	Day 1 A dose of 0.3 mL of a 10% concentration of test substance was placed on a Hilltop chamber backed by adhesive tape (occlusive patch) and applied to the clipped surface of test animals as quickly as possible. Day 7 and Day 13 The induction procedure was repeated.
Challenge procedure:	Day 27 Chambers containing a challenge dose of 1.25% concentration of test substance were applied to the trunks of test animals and secured for 20 hours with elastic wrap and tape. Approximately 20 hours after chamber removal for challenge, the test sites were depiliated. Approximately six hours after chamber application, the elastic wrap, tape, and chambers were removed. The test sites were graded for irritation at approximately 24 and 48 hours following chamber application at induction and at approximately 24 and 48 hours following chamber removal at challenge
Test method:	US EPA Series 81
Comment:	Following challenge with 1.25% w/v S10737.01, dermal scores of 0 (no reaction) to ± (slight patchy erythema) were noted in all test and challenge control animals. Group mean dermal scores were similar between the test and challenge control animals.
Result:	The analogue chemical was non-sensitising to the skin of guinea pigs.

9.2 A subchronic toxicity test with an analogue compound, xylene sulfonic acid sodium salt, in mice and rats. (Wheeler, 1980)

Species/strain:	Mouse/B6C3F1; rat/Fischer 344
Number/sex of animals:	10/sex/group; 5 groups for both species

Method of administration: Diet ad libitum;
diet levels 0.125%, 0.25%, 0.5%, 1.0% and 2%

Dose/Study duration: 91 days

Test method: Not stated

Clinical observations and other findings:

Mice
Mortality was limited to four mice, three males of the 0.5% level and one female of the lowest (0.125%) level. These deaths were not considered to be treatment related.
There was no clinical evidence of toxicity in any group. Body weights of both sexes fluctuated widely from week to week but by termination, any differences noted were considered to be due to normal variation. Pathological examinations did not reveal any gross or microscopic lesions that could be attributed to the treatment.

Rats
There were no significant differences between the body weights of the test groups and their controls and there were no clinical signs of toxicity in rats at any dose level.
There were no gross or microscopic lesions found that could be attributed to the test compound.

Comment: The analogue chemical was considered to produce no evidence of toxicity when fed to mice and rats at a high dose of 2% body weight (20 gm/kg) in the diet, for a period of 91 days.

Based on clinical signs and effects on body weight gain, the No Observed Effect Level (NOEL) is determined at 20 gm/kg/day.

Result: A NOEL of 20 gm/kg/day was established in this study.

9.3 Developmental toxicity

Only a summary report was provided for this study. Upon request the notifier indicated that the full study report was unavailable.

Species/strain: Charles River rats

Number/sex of animals: 4 groups of 30 females

Method of administration: daily by gavage

Dose/Study duration: 0, 150, 1 500 and 3 000 mg/kg/day on days 6 to 15 of gestation

Test method: US TSCA Health Effects Test Guidelines, 1995

Clinical observations and other findings:

Not stated

Result:	The notified chemical did not appear to be developmental toxicant at dose levels tested.

9.4 Genotoxicity

9.4.1 *Salmonella typhimurium* Reverse Mutation Assay (Page, 1994e)

Strains:	*Salmonella typhimurium* TA1535, TA1537, TA98 and TA100
Concentration range:	0, 100, 333, 1000, 3333, 5000 μg/plate, diluted in water
Metabolic activation:	10% rat liver S9 fraction (Aroclor 1254-induced) in standard cofactors
Positive controls:	TA98 + S9: 1 μg/plate 2-aminoanthracene TA98 – S9: 1μg/plate 2-nitrofluorene TA100 + S9: 1 μg/plate 2-aminoanthracene TA100 – S9: 1 μg/plate sodium azide TA1535 +S9: 1 μg/plate 2-aminoanthracene TA1535 – S9: 1 μg/plate sodium azide TA1537 + S9: 1 μg/plate 2-aminoanthracene TA1537 – S9: 75 μg/plate 9-aminoacridine
Test method:	Not available
Comment:	Neither precipitation nor appreciable toxicity was observed at the highest test concentration of 5000 μg/plate. All concentrations were tested in triplicate Under the conditions of the study, the notified chemical caused no substantial increases in revertant colony numbers over control counts at any concentration in either the presence or absence of the rat liver microsomal enzymes. All positive and negative controls responded appropriately.
Result:	The notified chemical was considered to be non-mutagenic under the conditions of the assay.

9.4.2 Micronucleus Assay in the Bone Marrow Cells of the Mouse (Putman, 1994)

Species/strain:	Mouse/ICR
Number and sex of animals:	5/sex/group
Doses:	0, 145, 290 and 580 mg/kg of test substance in deionised water; 40 mg/kg cyclophosphamide (positive control)
Method of administration:	IP injection at a constant volume of 20 mL/kg
Test method:	Not available
Comment:	No mortality was observed during the course of the study. Lethargy was noted in both sexes at the 580 mg/kg dose level. Respective groups were sacrificed at 24, 48 and 72 hours post-treatment for evaluation. There was a 36% reduction in the ratio of polychromatic erythrocytes in male mice sacrificed 72 hours following treatment with 580 mg/kg, relative to the vehicle controls, indicating the suitability of the dose levels selected for testing. No significant increases in micronucleated polychromatic erythrocytes in either sex of mice at 24, 48 or 72 hours after dose administration, relative to vehicle controls. Positive and negative controls responded appropriately.
Result:	The notified chemical was considered to be non-clastogenic under the conditions of the assay.

9.5 Skin Effects of Formulations Containing the Notified Chemical

A number of test protocols were used for testing the irritation potential of formulations containing the notified chemical together with other detergent ingredients. These formulations were diluted in many cases, to concentrations < 5%. These products were reported to be mildly irritating to non-irritating.

A number of Repeated Insult Patch Tests in humans using formulations containing the notified chemical were tabulated by the notifier. No evidence of contact sensitisation related to the notified chemical was observed.

A number of additional human tests on formulations, designed to support claims of "mildness" for the products, were tabulated by the notifier. These were mostly performed using concentrations ranging from normal use to ten times normal use. The evidence from the large number of studies is consistent with the irritation and sensitisation results reported above.

9.6 Overall Assessment of Toxicological Data

The notified chemical was of very low acute oral toxicity (LD_{50}=3346 mg/kg) in the rat and low acute dermal toxicity (LD_{50}>2000 mg/kg) in the rabbit. It was non-irritating to rabbit skin but produced mild signs of irritation in the rabbit eye. An inhalation study was not undertaken, as the notified chemical is an aqueous solution with a vapour pressure similar to water. Analogue data were provided to assess the skin sensitisation potential of the notified chemical. An analogue of the notified chemical was found not to be a skin sensitiser in a non adjuvant type test.

A number of skin irritation and sensitisation studies on humans have been performed using formulations containing the notified chemical. The notified chemical was found to be a slight skin irritant under the conditions of the tests, but not to be a skin sensitiser.

In genotoxicity studies, the notified chemical was not mutagenic in bacteria, nor did it induce an increased incidence of micronuclei in the bone marrow of mice.

Data relating to another analogue chemical, xylene sulfonic acid sodium salt, were provided for a subchronic toxicity study of 91 days duration. The analogue chemical was considered to produce no evidence of toxicity when fed to mice and rats at a high dose of 2% (20 gm/kg/day) body weight in the diet, for a period of 91 days. Based on this observation NOEL for the notified chemical was determined to be 20 gm/kg/day.

In a developmental toxicity study, the notified chemical was found to not cause developmental toxicity at doses up to 3 000 mg/kg/day.

Hazard Classification
Based on the above studies and analogue data, the notified chemical has a toxicology profile which appears to be below the threshold for health effects classification as a hazardous substance according to NOHSC *Approved Criteria for Classifying Hazardous Substances* [NOHSC, 1999b].

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

The notifier supplied the following ecotoxicity data in support of the application. The test data were generated according to OECD protocols.

AQUATIC TOXICITY DATA

Test	*Species*	*Results (measured)*
Acute Toxicity to Fish of [OECD 203]	Rainbow trout Oncorhynchus mykiss	LC50 (96 h) > 1,580 mg/L NOEC (96 h) = 824 mg/L
Acute Immobilisation to Fresh water invertebrates [OECD 202]	*Daphnia magna*	EC_{50} (48 h) >1,020 mg/L NOEC (48 h) = 470 mg/L
Inhibition of Algal growth [OECD TG 201]	*Selenastrum capricornutum*	E_bC_{50} (96 h) = 758 mg/L NOEC (96 h) = 240 mg/L

Fish

The tests on Rainbow trout were conducted using a flow through methodology, with solutions of the new chemical made up at nominal concentrations of 112, 224, 448, 895 and 1790 mg/L together with a control. The actual test concentrations of the chemical were measured at end of the 96 hour test period, and were always within always between 92 and 112% of the nominal concentrations. Each test was performed in duplicate, using 10 animals in each test vessel. Temperature was maintained at 12±1°C, and water hardness, pH and dissolved oxygen levels were around 145 mg/L (as $CaCO_3$), between 7.7 and 8.2 and always greater than 7.6 mg/L, respectively.

No fish mortality was observed over the entire test duration for any of the test concentrations. However, after only 24 hours exposure to the highest concentration (measured as 1580 mg/L) unusual appearance and distressed behaviour was observed in most of the fish in each of the duplicate vessels, and persisted over the full 96 hour test duration. These effects included a darkening of pigmentation, laboured respiration, surfacing and loss of equilibrium.

The data indicate that while the LC_{50} is in excess of 1580 mg/L, the NOEC is 824 mg/L (measured concentration). On the basis of these results, the chemical may be classified as practically non toxic to this fish species.

Invertebrates

An acute toxicity test of new chemical against *Daphnia magna* was conducted in a flow through test over a 48 hour period using one control and five test solutions made up at nominal concentrations of 0 (control), 60, 120, 250, 500 and 1,000 mg/L at a temperature maintained at 20 ± 1°C. The actual test concentrations were measured at the beginning and end of the 48 hour test period, and were respectively 39, 150, 220, 470 and 1020 mg/L. These values were usually within 25% of the nominal concentrations. The test was conducted in duplicate using 10 daphnia in each test vessel. During the tests the water hardness was around 152 mg/L (as $CaCO_3$), the pH between 8.2 and 8.5 and the dissolved oxygen levels between 7.5 and 7.9 mg/L. No mortality was observed over the 48 hour test period for the measured test concentrations of 220 mg/L and lower, but after 48 hours exposure at 470 mg/L one of the test animals was observed on the bottom of the test chamber, while after 48 hours exposure at the highest test concentration 40% of the animals were observed on the bottom.

The data was analysed using the methods of Stephan et al. (1978) to provide the results tabulated above. These data indicate that the new chemical is practically non toxic to this species of daphnia.

Algae

Tests on algal growth inhibition were also performed with solutions of the new compound made up in nutrient media at nominal concentrations of 0 (control), 62.5, 125, 250, 500 and 1,000 mg/L, and three replicate tests were conducted at each concentration over a 96 hour test period. The actual test concentrations were measured at the beginning and end of the 96 hour test period, and were respectively 60.1, 122, 240, 483 and 980 mg/L. These values were always within 5% of the nominal concentrations. The mean temperature throughout the test was 24.5±0.5°C, and the pH of the media containing algae was observed to rise slightly with time from 7.4 at the beginning of the test to 7.9 after 4 days. Growth of algal biomass was monitored by counting the cell density (coulter counter) over the 96 hour test period, and appropriate data used for the construction of growth curves. Inhibition of algal growth (after 96 hours) was observed for all test concentrations in excess of 122 mg/L, but the data analysed using Dunnett's test indicated that inhibition was significant only for test concentrations greater than the (measured) No Observed Effect Concentration (NOEC) of 240 mg/L. The analysis indicated that the 96 hour E_bC_{50} = 758 mg/L. These results indicate that the new chemical is practically non toxic to this species of green algae.

Sewage Bacteria

No data was submitted on the effects of the new chemical on bacterial respiration, but the high rates of biodegradation encountered in both the Modified Sturm Test and the Modified SCAS test (see above) indicate that no significant toxic effects were observed to bacteria exposed to the new chemical at concentrations up to 20 mg/L equivalent of organic carbon.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

The new chemical is to be used as a stabiliser in domestic dishwashing formulations, and almost all (around 66 tonnes per annum) is expected to be released to the sewer system. Although it does not meet the criteria for "ready biodegradability" as defined in OECD TG 301B, the chemical has been shown to be rapidly and extensively degraded under aerobic conditions, including in tests designed to simulate an activated sludge sewage treatment plant.

The chemical is at worst practically non toxic to those aquatic species against which it has been tested, with an LC_{50} for green algae (the most sensitive species) determined as 758 mg/L.

The new chemical will be used throughout Australia, and consequently an estimate of the Predicted Environmental Concentration (PEC) may be made on a "global" basis.

The following PEC calculation assumes that the dishwashing formulations containing the surfactant are used nationwide, and that all is released to the sewer system. It is also assumed that 150 L of sewerage are generated each day by each person. Due to the very high water solubility, almost all the new compound is expected to remain in the water column.

Import rate	66 tonne per annum
Release rate	66 tonne per annum
Population (national)	18,000,000
Volume of sewerage per annum	18.000,000,x 365 x150
	= 985 x 10^9 L per annum

Mean concentration in sewerage 67 μg/L

On release to receiving waters (after treatment at the sewage treatment plant), it is usually assumed that the effluent is diluted by a factor of 10. This gives a final PEC of 6.7 μg/L.

In the unlikely event of all the product being used in a single major city, with populations of around 3,000,000, the mean concentration in the sewerage would be 428 μg/L, which would be diluted to 42.8 μg/L on release to receiving waters.

The calculation above assumes that no biodegradation of the compound occurs in the sewage treatment plants prior to discharge to receiving waters. In fact it is likely that most of the chemical will have been destroyed prior to discharge, and so the calculations above are a worst case scenario. However, even assuming no biodegradation, the estimated PECs are at least four orders of magnitude below levels which have been shown to be toxic to aquatic organisms.

The chemical is assessed as having low potential for bioaccumulation. The chemical is not expected to have affinity for the organic component of soils or sediments, and the high water solubility indicates that it would be mobile in these media.

It is concluded that the new chemical presents a low hazard to the environment when used as a component of dishwashing liquid as indicated by the notifier.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

The notified chemical is not determined to be a hazardous, according to the NOHSC Approved Criteria for Classifying Hazardous Substances (NOHSC, 1999b).

The acute oral toxicity of the notified chemical is very low (LD_{50}= 3346 mg/kg) and the acute dermal toxicity is low (LD_{50}>2 000 mg/kg). It is neither a skin irritant in rabbits nor a skin sensitiser. It was a slight irritant to rabbit eye and skin of humans. No evidence of genotoxicity was observed in one *in vitro* and another *in vivo* genotoxicity tests. The notified chemical was not determined to be a developmental toxicant in rats (full study report not available – based on summary report only).

For longer term systemic effects, in a 91 day feeding study using an analogue in mice and rats, there was no evidence of toxicity. The NOEL was determined at 20 gm/kg/day.

Occupational Health and Safety

Occupational exposure to the notified chemical prior to end use is expected to be negligible, as it will be imported as a component of a formulated dishwashing liquid, and will not require formulation or repackaging in Australia. The health risk for transport, storage and retail workers is expected to be negligible unless packaging is breached. Little exposure is expected when cleaning up spills because the notified chemical will be present at a concentration of 3.41% in the imported product and workers are expected to wear coats and gloves.

Wash-up workers in commercial premises may be exposed to the chemical, but the risk would be similar to that of the public.

Public Health
As the notified chemical will be used in a washing liquid, there will be widespread dermal exposure to the public, limited only by the commercial success of the product. Systemic exposure from dermal contact with notified chemical in dishwashing liquid is calculated using reference values from Risk Assessment of Existing Substances: Technical Guidance Document (European Commission, 1994).

The dishwashing liquid "Dawn" containing 3.41% of the notified chemical would result in a systemic exposure of 0.036 mg/kg/day, based on the following assumptions.

volume used per application = 10 g
fraction remaining on the skin = 5 %
weight fraction of notified chemical = 3.41 %
dermal absorption = 10 %
frequency of use = 3 times per day, every day
body weight = 60 kg

In comparison with the NOEL of 2% or 20 g/kg/day established in the 91-day toxicity study in mice and rats, the above estimated exposure would represent a safety margin of greater than 230000 for the notified chemical in this product.

The notified chemical is a slight eye irritant but not a skin irritant at 31.2%. The hazard associated with slight eye irritancy is likely to be offset by the low concentration (maximally 3.41 % and likely to be considerably less once diluted in water) and use pattern (predominantly dermal exposure via the hands, which could be considerably reduced by the wearing of rubber gloves) of the notified chemical. Consequently, the potential hazard from the use of the notified chemical is considered to be low. There will be minimal public exposure from transport and storage.

Based on the submitted information, it is considered that calcium xylene sulphonate will not pose a significant hazard to public health when used in the proposed manner.

13. RECOMMENDATIONS

To minimise occupational exposure to calcium xylene sulphonate the following guidelines and precautions should be observed:

- Industrial clothing should conform to the specifications detailed in AS 2919 (Standards Australia, 1987) and AS 3765.2 (Standards Australia, 1990); impermeable gloves should conform to AS/NZS 2161.2 (Standards Australia, 1998); all occupational footwear should conform to AS/NZS 2210 (Standards Australia/Standards New Zealand, 1994);

- Spillage of the notified chemical should be avoided. Spillages should be cleaned up promptly with absorbents which should be put into containers for disposal;

- Good personal hygiene should be practised to minimise the potential for ingestion;
- A copy of the MSDS should be easily accessible to employees.

14. MATERIAL SAFETY DATA SHEET

The MSDS for the notified chemical was provided in a format consistent with the *National Code of Practice for the Preparation of Material Safety Data Sheets* (NOHSC, 1994).

This MSDS was provided by the applicant as part of the notification statement. It is reproduced here as a matter of public record. The accuracy of this information remains the responsibility of the applicant.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the Act, secondary notification of the notified chemical shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

Greater exposure to the public may occur if the concentration of notified chemical in the product is increased, or if additional products containing the notified chemical enter the public domain. In these circumstances, secondary notification may be required to assess the hazards to public health.

16. REFERENCES

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Attachment 1

The Draize Scale for evaluation of skin reactions is as follows:

Erythema Formation	*Rating*	*Oedema Formation*	*Rating*
No erythema	0	No oedema	0
Very slight erythema (barely perceptible)	1	Very slight oedema (barely perceptible)	1
Well-defined erythema	2	Slight oedema (edges of area well-defined by definite raising	2
Moderate to severe erythema	3	Moderate oedema (raised approx. 1 mm)	3
Severe erythema (beet redness)	4	Severe oedema (raised more than 1 mm and extending beyond area of exposure)	4

The Draize scale for evaluation of eye reactions is as follows:

CORNEA

Opacity	*Rating*	*Area of Cornea involved*	*Rating*
No opacity	0 none	25% or less (not zero)	1
Diffuse area, details of iris clearly visible	1 slight	25% to 50%	2
Easily visible translucent areas, details of iris slightly obscure	2 mild	50% to 75%	3
Opalescent areas, no details of iris visible, size of pupil barely discernible	3 moderate	Greater than 75%	4
Opaque, iris invisible	4 severe		

CONJUNCTIVAE

Redness	*Rating*	*Chemosis*	*Rating*	*Discharge*	*Rating*
Vessels normal	0 none	No swelling	0 none	No discharge	0 none
Vessels definitely injected above normal	1 slight	Any swelling above normal	1 slight	Any amount different from normal	1 slight
More diffuse, deeper crimson red with individual vessels not easily discernible	2 mod.	Obvious swelling with partial eversion of lids	2 mild	Discharge with moistening of lids and adjacent hairs	2 mod.
		Swelling with lids half-closed	3 mod.		
Diffuse beefy red	3 severe	Swelling with lids half-closed to completely closed	4 severe	Discharge with moistening of lids and hairs and considerable area around eye	3 severe

IRIS

Values	*Rating*
Normal	0 none
Folds above normal, congestion, swelling, circumcorneal injection, iris reacts to light	1 slight
No reaction to light, haemorrhage, gross destruction	2 severe