File No: NA/477

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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

Polymer in MCP 1517

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT

Polymer in MCP 1517

1. APPLICANT

Bentley Chemplax Pty Ltd of 110 Drummond Street OAKLEIGH VIC 3166 and Mobil Oil Australia Limited of 417 St Kilda Road MELBOURNE VIC 3004 have submitted a limited notification statement in support of their application for an assessment certificate for Polymer in MCP 1517.

2. IDENTITY OF THE CHEMICAL

MCP 1517 is not considered to be hazardous based on the nature of the chemical and the data provided. Therefore the chemical name, CAS number, molecular and structural formulae, molecular weight, spectral data, details of the polymer composition and details of exact import volume and customers have been exempted from publication in the Full Public Report and the Summary Report.

Trade name:	MCP 1517
Other name:	none known
Method of Detection and Determination:	infrared spectroscopy has been used to characterise the polymer

MCP 1517 contains 30% of the notified polymer in petroleum distillate. The notified material is a condensation product of a 2,5-furandione moiety substituted with a polyisobutylene (of MW around 840 $g.mol^{-1}$) with ethanol, 2-(diethylamino). It is amphoteric with a zwitterionic head group formed as a result of the condensation reaction. The polydispersity in the notified material is a consequence of a distribution in chain lengths in the polyisobutylene portion of the material, which (for the production batch for which the notifier supplied information) has a NAMW of
963 $g.mol^{-1}$ and a polydispersity of 1.47.

In respect of the overall composition of the material, it is difficult to reconcile the 5 to 45% stated weight range for the ethanol, 2-(diethylamino) component which occurs only once in each molecule. Based on the structural formula, and taking the NAMW of the polyisobutylene moiety as 963 $g.mol^{-1}$, the calculated percentage of this component would be expected to be around 10%. The highest weight percent (45%) for this component indicated in the notification could only be valid if the polyisobutylene chains were very much smaller than stated in the notification.

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	non-volatile, amber liquid with mild odour
Boiling Point:	not available
Specific Gravity:	0.91
Vapour Pressure:	not available
Water Solubility:	< 1%
Partition Co-efficient (n-octanol/water):	log P_{ow} > 7 (calculated value) (1)
Hydrolysis as a Function of pH:	not available
Adsorption/Desorption:	not available
Dissociation Constant:	not available
Flash Point:	141°C
Flammability Limits:	not available
Autoignition Temperature:	not available
Explosive Properties:	not available
Reactivity/Stability:	not available

Comments on Physico-Chemical Properties

The notified material is a powerful emulsifying agent specially suited to the stabilisation of water in oil emulsions. As such, the effectiveness of the material depends on it having negligible true water solubility, although the formation of colloidal aggregated structures such as micelles may be possible. The polymer contains a large branched chain aliphatic hydrocarbon coupled to a polar end group, and as such is amphoteric in nature. This constitution indicates that the material will have powerful surfactant properties.

The material is likely to have a low vapour pressure under normal environmental conditions.

The low water solubility means that direct determination of the octanol/water partition coefficient would be difficult. However, the notifier supplied details of an estimated calculation for log P_{ow} based on an accepted methodology. This

calculation gave an estimated log P_{ow} greater than 7, which indicates the material would partition into the oil phase and would bind strongly to the organic component of soils and sediments.

Several physio-chemical property tests of the notified polymer were not performed.

No data on hydrolytic degradation was provided. The material contains an ester linkage which could be susceptible to hydrolysis under extremely high or low conditions of pH. However, the low water solubility indicates that hydrolysis would be very slow under usual environmental pH conditions of between 4 and 9.

No dissociation constant data was provided, but the zwitterionic head group could be expected to make the molecule cationic under conditions of low pH (pH<4) and anionic at high pH (>11). In the normal environmental pH range the material is expected to be neutral, with the positive and negative charges balanced.

4. PURITY OF THE CHEMICAL

Toxic or Hazardous Impurities:

Chemical name:	2-diethylaminoethanol
CAS No.:	100-37-8
Weight percentage:	< 4%
Toxic properties:	moderately toxic by ingestion or skin contact; a severe eye and mild skin irritant (2)

5. OCCUPATIONAL EXPOSURE

The notified substance will be imported in sealed iso-containers and distributed to industrial plants for blending into mining explosives. During the blending process, MCP 1517 will be transferred directly from the iso-containers to the blend tank by a pump and hoses. The finished products will be transferred to large tanks and delivered to mining sites by trucks. At mining sites, the formulated explosive will be pumped directly into the blast hole from tank trucks. The operator at the mine site will take a sample prior to loading to check product quality. When exploded, the notified chemical will be combusted to carbon dioxide, water and nitrogen. Worker exposure to MCP 1517 during the transfer, formulation and end use is considered to be low. Workers at the mine sites are most likely to be exposed to the notified chemical. The most likely route of exposure would be dermal contamination.

The tanks used for transport are typically dedicated to this type of service and any associated residue does not get washed out until the truck carries a non-compatible material. The hoses are also dedicated equipment and not washed between usages.

6. PUBLIC EXPOSURE

The notified chemical will not be sold to the public and no public exposure is expected from the industrial use.

Residual materials in the iso-containers, blending equipment and truck will be washed out and passed to waste water treatment facilities. Public exposure from disposal is anticipated to be negligible. Accidental spills will be contained with absorbent materials, which are expected to be disposed of to licensed waste disposal sites according to government regulations.

7. ENVIRONMENTAL EXPOSURE

Release

Production of the explosive emulsion will take place in batching plants operated at a number of locations near mines/quarries throughout Australia. The final emulsion which contains around 1.2% of the notified material, is transferred to dedicated tank trucks and transported to the various sites of blasting activity at mines and quarries. The emulsion is pumped directly from the tankers into pre-drilled blast holes, and is detonated through the use of electrically initiated blasting caps.

Typically the blast holes in quarries are 5 to 23 cm wide and 6 to 8 metres deep, while in open pit mining operations the holes are 25 to 38 cm in diameter and 12 to 18 metres deep. These dimensions correspond to hole (and hence explosive) volumes of 0.012 m^3 to 2.04 m^3.

Losses of the material during formulation are expected to be very low, and residual emulsion (containing around 0.5-2% of the notified material) left in the blending tanks would be diluted with water and passed to on site waste water treatment plants. Residual material remaining in the iso-containers would also be passed to these facilities following cleaning of the containers.

The production process involves two transfer operations of the fuel oil/notified material solution, and major release of the notified chemical during emulsion production is likely to occur only in the event of accident. In this event spills would be contained by the bunding and then treated at the on site waste water treatment plants.

Fate

The residual notified chemical passed onto waste water treatment plants as a result of cleaning equipment used for emulsion production will become assimilated with the sludge, and would presumably then be disposed of to landfill, or perhaps be incinerated. The notified material is not readily biodegradable (see below), but in a landfill could be expected to undergo slow degradation to carbon dioxide or methane, water and small amounts of nitrogen or ammonia. Incineration would destroy the material with production of water vapour, and oxides

of carbon and nitrogen.

When the explosive emulsion is detonated, the material could be expected to be destroyed immediately, again producing oxides of carbon and nitrogen.
The notified material is not readily biodegradable, and tests equivalent to the modified Sturm test (3) indicated that only around 9% of the notified material was degraded after 28 days. Under the same conditions 84% of a control material, sodium benzoate, had degraded after the 28 day period.

The material has a relatively high molecular weight (NAMW =1,060 $g.mol^{-1}$) with a very high value for log K_{ow} (>7), and consequently it could be expected to have low bioaccumulation potential.

8. EVALUATION OF TOXICOLOGICAL DATA

The toxicological data submitted by the notifier were generated from MCP 1517 which contains 30% of the notified polymer and are summarised below.

8.1 Acute Toxicity

Summary of the acute toxicity of MCP 1517

Test	*Species*	*Outcome*	*Reference*
acute oral toxicity	rat	LD_{50} > 2 000 $mg.kg^{-1}$	(4)
acute dermal toxicity	rat	LD_{50} > 2 000 $mg.kg^{-1}$	(5)
skin irritation	rabbit	slight irritant	(6)
eye irritation	rabbit	moderate irritant	(7)

8.1.1 Oral Toxicity (4)

Species/strain:	rat/Spague-Dawley
Number/sex of animals:	5/sex
Observation period:	14 days
Method of administration:	MCP 1517 in Mazola corn oil (50%, w/w) was administered orally
Clinical observations:	no signs of systemic toxicity were noted
Mortality:	none
Morphological findings:	no gross pathological changes were noted at necropsy

Test method:	USEPA Guidelines (8)
LD_{50}:	> 2 000 $mg.kg^{-1}$
Result:	MCP 1517 was of low acute oral toxicity in rats

8.1.2 Dermal Toxicity (5)

Species/strain:	rabbit/New Zealand White
Number/sex of animals:	5/sex
Observation period:	14 days
Method of administration:	MCP 1517 was applied to the shaved back of each animal and the test site was covered by 8-ply gauze followed by a rubber dam and surgical tape; the test site was wiped clean after patch removal 24 hours later
Clinical observations:	no signs of systemic toxicity were noted
Mortality:	none
Morphological findings:	no gross pathological changes were noted at necropsy
Test method:	USEPA Guidelines (8)
LD_{50}:	> 2 000 $mg.kg^{-1}$
Result:	MCP 1517 was of low acute dermal toxicity in rabbits

8.1.3 Inhalation Toxicity

Inhalation toxicity study was not provided as it is a limited notification.

8.1.4 Skin Irritation (6)

Species/strain:	rabbit/New Zealand White
Number/sex of animals:	3/sex
Observation period:	76 hours

Method of administration: MCP 1517 (0.5 mL) was applied to a 1 square inch shaved area on the anterior and posterior flanks of each animal; the test sites were occluded with Webril patches and secured with a rubber dam and surgical tape; anterior patches were removed after 1 hour for corrosion test and after 4 hours for irritation test; test sites were wiped clean after patch removal

Draize scores (9):

Time after treatment (days)	***Animal #***		
	1	***2***	***3***
Erythema			
1	1[a]	1	0
2	1	1	0
3	0	0	0
4	1	0	0
5	1	1	0
6	1	1	0
Oedema			
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	1	0	0
6	1	0	0

[a] see Attachment 1 for Draize scales

Test method: USEPA Guidelines (8)

Result: both 1 and 4 hour occluded test sites showed no ulceration or necrosis immediately after patch removal or at 48 hours; MCP 1517 was a slight skin irritant in rabbits

8.1.5 Eye Irritation (7)

Species/strain: rabbit/New Zealand White

Number/sex of animals: 3/sex

Observation period: 6 days

Method of administration: MCP 1517 (0.1 mL) was instilled into the left conjunctival sac of each animal and the eyelids gently held together for 1 second; all test sites were stained with fluorescein during the 24 hour evaluation

Draize scores (9) of unirrigated eyes:

	Time after instillation								
Animal	**1 day**			**2 days**			**3 days**		
Cornea	**o[a]**	**a[b]**		**o[a]**	**a[b]**		**o[a]**	**a[b]**	
1	0[1]	0		0	0		0	0	
2	1	1		0	0		0	0	
3	0	0		0	0		0	0	
4	0	0		0	0		0	0	
5	1	1		0	0		0	0	
6	0	0		0	0		0	0	
Conjunctiva	**r[c]**	**c[d]**	**d[e]**	**r[c]**	**c[d]**	**d[e]**	**r[c]**	**c[d]**	**d[e]**
1	3	1	2	1	0	0	1	0	0
2	3	2	1	2	1	0	2	0	0
3	2	1	1	2	1	0	2	1	0
4	2	1	1	1	1	0	1	0	0
5	2	1	1	1	1	0	1	0	0
6	2	1	0	1	0	0	1	0	0

[1] see Attachment 1 for Draize scales
[a] opacity [b] area [c] redness [d] chemosis [e] discharge

Irritated eyes: Draize scores for iris lesions were zero in all the animals; moderate corneal irritation and moderate to severe conjunctival irritation were noted at 1 hour and diminished over the remainder of the study, corneal ulcerations were noted in the three animals at 24 hours post-dosing; these ulcerations were healed at the 48-hour evaluation

Test method: USEPA Guidelines (8)

Result: MCP 1517 was a moderate eye irritant in rabbits

8.1.6 Skin Sensitisation

Skin sensitisation study was not provided as it is a limited notification.

8.2 Repeated Dose Toxicity

Repeated dose toxicity study was not provided as it is a limited notification.

8.3 Genotoxicity

8.3.1 *Salmonella typhimurium* Reverse Mutation Assay (10)

Strains:	TA 98, TA 100, TA 1535, TA 1537 and TA 1538
Concentration range:	0.003 to 10 μL/50 μL tetrahydrofuran per plate
Test method:	USEPA Guidelines (8)
Result:	MCP 1517 was not a mutagen with or without metabolic activation in the Ames test

8.3.2 Micronucleus Assay in the Bone Marrow Cells of the Mouse

The study of micronucleus assay in the bone marrow cells of the Mouse was not provided as it is a limited notification.

8.4 Overall Assessment of Toxicological Data

MCP 1517, containing 30% the notified chemical, is of low acute oral toxicity in rats (LD_{50} > 2 000 $mg.kg^{-1}$) and low acute dermal toxicity in rabbits (LD_{50} > 2 000 $mg.kg^{-1}$). When tested in rabbits, it is a slight skin and moderate eye irritant. In the presence or absence of metabolic activation, MCP 1517 was not mutagenic in bacteria. No studies on skin sensitisation, repeat dose toxicity or micronucleus assay in mouse bone marrow cells were provided.

On the basis of submitted data, MCP 1517 would not be classified as hazardous in accordance with Worksafe Australia's *Approved Criteria for Classifying Hazardous Substances (11)* in relation to acute lethal effects (oral, dermal) or irritancy effects (skin, eye).

9. ASSESSMENT OF ENVIRONMENTAL EFFECTS

Although not required for polymeric material with NAMW greater than 1 000, the following ecotoxicity studies have been supplied by the notifier.

Test	Species	Results (Nominal)
Acute Toxicity (freshwater fish)	Rainbow Trout *Oncorhynchus mykiss*	LC_{50} (96 h) >5 000 mg.L^{-1}
Acute Toxicity (saltwater fish)	Sheepshead Minnow (*Cyprinodon variagatus*)	LC_{50} (96 h) >2 000 mg.L^{-1}
Acute Toxicity (saltwater invertebrate)	Mysid Shrimp (*Mysidopsis bahia*)	LC_{50} (96 h) >5,000 mg.L^{-1}

The ecotoxicity tests for rainbow trout and sheepshead minnow were conducted according to OECD test guidelines with nominal concentrations of the nominated substance of 100, 500, 1 000, 2 000 and 5 000 mg.L^{-1} introduced into the test chambers as an oil in water emulsion at the beginning of each test. For the duration of all static tests the (water insoluble) notified material was kept in suspension through mechanical agitation.

The ecotoxicity data for the notified polymer indicates that the material is non toxic to rainbow trout. During the tests there was slight mortality among the test specimens, and 15% had died at the end of the 96 hour test period following exposure to 5 000 mg.L^{-1} of the test substance. It was not possible to determine a NOEC due to turbidity in the water during the tests.

Acute toxicity tests were also conducted on sheepshead minnow (*Cyprinodon variagatus*). No mortality was observed during the test duration, and the data was such that the LC_{50} was determined as greater than 2 000 mg.L^{-1}, and consequently the material may be regarded as slightly toxic to this species.

Although not specified in OECD test guidelines for ecotoxicity, tests on mysid shrimp (*Mysidopsis bahia*), a representative marine invertebrate, are recognised by the US EPA, and were conducted for the notified polymer. In this study the shrimps were exposed to the water soluble fraction (WSF) of the notified material derived from quantities of the test material calculated to give nominal exposures of 103, 513, 1 026, 2 053 and 5 038 mg.L^{-1}. Insignificant mortality occurred throughout the test period and no deaths occurred with either the control (0 mg.L^{-1}) or the highest nominal concentration (5 038 mg.L^{-1}). The notified material is therefore regarded as not toxic to this species with a LC_{50} greater than 5 000 mg.L^{-1}. No abnormal behaviour of the test specimens was observed, and consequently the NOEC was also determined as greater than 5 000 mg.L^{-1}.

In all cases the exact extent of exposure is unclear. In the fish tests, using oil in water dispersions, the polymer was non toxic up to the limit of its solubility. The water soluble fractions in the mysid shrimp tests were also non toxic.

10. ASSESSMENT OF ENVIRONMENTAL HAZARD

The environmental hazard from the notified polymer is considered to be low. Release into the environment during production of the explosive emulsions will be small, and if released in wastewater would be incorporated into sludge and then incinerated or placed into landfill. Incineration would destroy the material with production of carbon and nitrogen oxides, and slow decomposition in a landfill

would be expected. The material is very hydrophobic, and any in the event of accidental spills would be expected to be adsorbed onto and become associated with the organic components of soils and sediments.

When used as indicated by the notifier, most of the material would be destroyed as a consequence of its incorporation into explosives.

The notified polymer is not likely to present a hazard to the environment when it is stored, transported and used in the typical manner.

11. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

The toxicological studies provided by the notifiers suggested that the notified chemical is likely to exhibit low toxicity via acute oral or dermal routes in humans. The chemical may cause moderate eye and slight skin irritation in the event of occupational exposure. As the polymer vapour pressure is expected to be low, inhalation exposure is unlikely. In addition, effects through dermal absorption are unlikely due to the high molecular weight.

The exposure for transportation workers and formulators is expected to be low. The work will be carried out in well ventilated areas at room temperature. They may be exposed to the notified chemical via dermal contact while connecting and disconnecting hoses. Eye contamination to the notified chemical could happen only in the event of accident.

The end users at the mine sites can be exposed to the notified chemical when taking assay samples and filling it into the blast holes. Dermal contact will be the main exposure route. Eye contamination is possible only when splashes occur. Considering the finished product contains 1.2% of the notified chemical, the risk for dermal and eye irritation to end users is expected to be minor.

No public exposure is expected from the industrial use. Residual materials in the containers and blending equipment will be washed out and treated in waste water treatment facilities. Public exposure from disposal is anticipated to be negligible. Should an accidental spillage occur, public exposure would be minimised by the emergency procedures described by the notifier, ie. contained with absorbent materials and disposed of according to government regulations.

12. RECOMMENDATIONS

To minimise occupational exposure to Polymer in MCP 1517 the following guidelines and precautions should be observed:

- Safety goggles should be selected and fitted in accordance with Australian Standard (AS) 1336 (12) to comply with Australian/New Zealand Standard (AS/NZS) 1337 (13);

- Industrial clothing should conform to the specifications detailed in AS 2919 (14) and AS 3765.1 (15);
- Impermeable gloves or mittens should conform to AS 2161 (16);
- All occupational footwear should conform to AS/NZS 2210 (17);
- Spillage of the notified chemical should be avoided, spillages should be cleaned up promptly with absorbents which should then be put into containers for disposal;
- Good personal hygiene should be practised to minimise the potential for ingestion;
- A copy of the Material Safety Data Sheet (MSDS) should be easily accessible to employees.

13. MATERIAL SAFETY DATA SHEET

The MSDS for the notified chemical was provided in accordance with the *National Code of Practice for the Preparation of Material Safety Data Sheets* (18).

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.

14. 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.

15. REFERENCES

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2. Lewis Sr R J, Sax N I & Lewis R J 1996, *Sax's Dangerous Properties of Industrial* Materials *(9th ed),* Van Nostrand Reinhold, New York.
3. Organisation for Economic Co-operation and Development, *OECD* Guidelines *for Testing of Chemicals,* OECD, Paris, France
4. Rodriguez S C *et al*. 1994, *Study No 65961*, *Acute oral toxicity of MCP 1517 in the Spague-Dawley rat*, Stonybrook Laboratories Inc, Princeton, NJ, USA.
5. Rodriguez S C *et al*. 1994, *Study No 65962*, *Acute dermal toxicity of MCP 1517 in the New Zealand White rabbit*, Stonybrook Laboratories Inc, Princeton, NJ, USA.

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16. Standards Australia 1978, *Australian Standard 2161-1978, Industrial Safety Gloves and Mittens (excluding electrical and medical gloves),* Standards Association of Australia Publ., Sydney.
17. Standards Australia/Standards New Zealand 1994, *Australian/New Zealand Standard 2210-1994, Occupational Protective Footwear*, Standards Association of Australia Publ., Sydney, Standards Association of New Zealand Publ, Wellington.
18. National Occupational Health and Safety Commission 1994, *National Code of Practice for the Preparation of Material Safety Data Sheets* [NOHSC:2011 (1994)], Australian Government Publishing Service, Canberra.

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.
Diffuse beefy red	3 severe	Swelling with lids half-closed	3 mod.	Discharge with moistening of lids and hairs and considerable area around eye	3 severe
		Swelling with lids half-closed to completely closed	4 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