

File No: NA/89

Date: 3/11/99

**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION
AND ASSESSMENT SCHEME**

FULL PUBLIC REPORT

**[3-(METHACRYLOYL AMINO) PROPYL] TRIMETHYLAMMONIUM CHLORIDE,
POLYMER WITH N-VINYL-2-PYRROLIDONE**

GAFQUAT HS-100

This Assessment has been compiled in accordance with the provisions of *the Industrial Chemicals (Notification and Assessment) Act 1989* 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 Arts, Sport, the Environment and Territories and the assessment of public health is conducted by the Department of Health, Housing and Community Services.

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT**[3-(METHACRYLOYL AMINO) PROPYL] TRIMETHYLAMMONIUM CHLORIDE,
POLYMER WITH N-VINYL-2-PYRROLIDONE****1. APPLICANT**

ISP (Australasia) Pty Limited, 73 - 75 Derby St, Silverwater,
NSW, 2141

2. IDENTITY OF THE CHEMICAL

Chemical name: [3-(Methacryloyl amino) propyl]
trimethylammonium chloride, polymer with N-
Vinyl-2-pyrrolidone

Chemical Abstracts Service

(CAS) Registry No.: 131954-48-8

Other name(s): Vinylpyrrolidone [3-(Methacryloyl amino)
propyl] trimethylammonium chloride

Vinylpyrrolidone methacrylamide
propyltrimethyl ammonium chloride

Vinylpyrrolidone MAPTAC

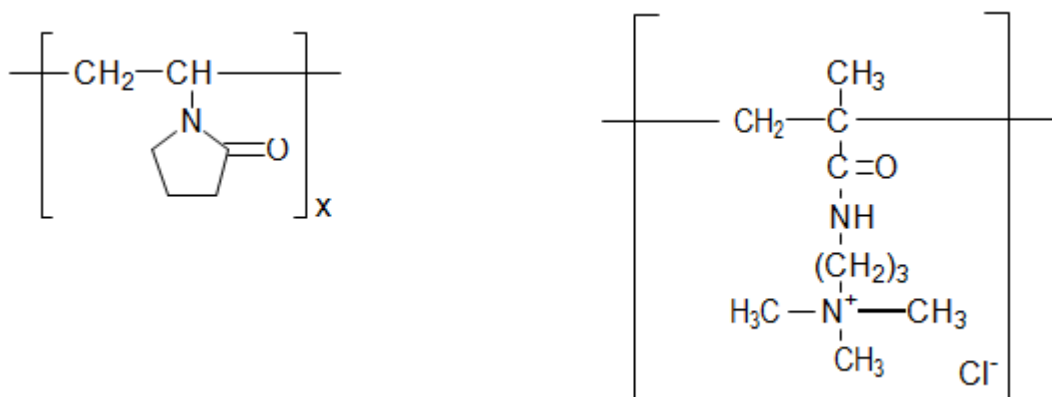
Agent AT-1269

Polyquaternium-28

Trade name(s): GAFQUAT HS-100

Molecular formula: $(C_6H_9NO)_x \cdot (C_9H_{21}N_2OCl)_y$

Structural formula:



Molecular weight:

Number-average molecular weight: >1000

Maximum percentage of low molecular weight species (molecular weight < 1000): <1.0%

Monomer(s) :

Chemical name:	1-Ethenyl-2-pyrrolidinone
Synonym(s) :	N-Vinyl-pyrrolidone
CAS No.:	88-12-0
Chemical name:	[3-(Methacryloyl amino) propyl]trimethylammonium chloride
Synonym(s) :	MAPTAC

Method of detection and determination:

Gel Permeation Chromatography, IR and NMR spectra, Microwave solids analysis

Spectral data:

The NMR and IR spectra were consistent with structure

3. PHYSICAL AND CHEMICAL PROPERTIES

As the polymer, "Agent AT-1269", is only ever used in an aqueous solution and as such will be imported as "GAFQUAT HS-100" (see section 5 below), the physical and chemical properties of GAFQUAT HS-100 are given here except where noted.

Appearance at 20°C and 101.3 kPa:	Hazy, highly viscous liquid
Glass-transition Temperature:	177°C (Agent AT-1269)
Specific Gravity/Density:	1050 kg/m ³
Water Solubility:	Freely soluble (Agent AT-1269)
Partition Co-efficient (n-octanol/water) log P_{O/W}:	<-1.2 at 20°C
Hydrolysis as a function of pH:	After 3 months storage: pH 7, Room Temp: 7.2% of MAPTAC hydrolysed pH 7, 45°C: 11.2% of MAPTAC hydrolysed pH 10, 45°C: 17% of MAPTAC hydrolysed
Adsorption/Desorption:	K _{OC} = 1653 (oc = organic carbon)

Dissociation Constant

The quaternary ammonium group is 100% ionised in water and therefore has an infinitely small pK value (similar to NaCl). The amide group from the MAPTAC precursor behaves as a weak base. However, it cannot be directly titrated due to solubility limitations of the polymer in non-aqueous solvents. Comparison of this amide structure with similar low molecular weight model compounds suggests that the pK_b of the amide linkage in Gafquat HS-100 is probably >11.

Flash Point:	Not applicable for aqueous solution
Flammability Limits:	"
Combustion Products:	"
Pyrolysis Products:	"
Autoignition Temperature:	"
Explosive Properties:	"
Reactivity/Stability:	Incompatible with strong oxidising and reducing agents

4. PURITY OF THE CHEMICAL

Degree of purity: >99%

Maximum content of residual monomer(s): <1%

5. INDUSTRIAL USE

GAFQUAT HS-100 is to be imported as a 20% aqueous solution of the polymer, Agent AT-1269, to be marketed to the cosmetic manufacturing industry as a hair conditioning polymer for use in hair care products.

The estimated import quantity is 5 tonnes per annum.

6. OCCUPATIONAL EXPOSURE

GAFQUAT HS-100 will be imported as a 20% aqueous solution of Agent AT-1269 in sealed drums. It will be reformulated at approximately 10 sites involving approximately 170 workers.

GAFQUAT HS-100 is mixed with water and other water phase ingredients such as moisturisers, emulsifiers and preservatives and heated to 70°C. An oil phase of waxes, emollients and emulsifiers is also heated to about 70°C. The two phases are then

combined and emulsified with a high shear homogeniser and cooled to about 40°C when the perfume is added and mixed in.

Exposure to the notified chemical is mainly expected to result from pouring the viscous liquid into buckets for weighing and from filling of containers involved in heating and mixing. Because the polymer solution is viscous, the potential for spillage is limited.

During reformulation, care is taken not to aerate the solution during emulsification so that, although the mixers are not generally enclosed, a mist is not likely to be produced.

7. PUBLIC EXPOSURE

Because GAFQUAT HS-100 is to be used in the manufacture of hair care products, considerable public exposure may be expected. However, such products will generally contain only 5% GAFQUAT HS-100 (equivalent to 1% of the polymer). The notifier has estimated the exposure to the polymer to be less than 0.2 g per use.

GAFQUAT HS-100 is manufactured abroad and will be transported in Australia in labelled drums. Release to the environment at reformulation sites will be low (see below) and therefore public exposure from this source is expected to be minimal.

8. ENVIRONMENTAL EXPOSURE

. Release

The polymer will be compounded into cosmetics by an estimated 10 cosmetics manufacturing companies in at least 3 major cities and is expected to be sold Australia-wide providing a wide environmental exposure of the substance. Given that cosmetics formulation involves use of a maximum estimated import quantity of 5 tonnes per year of GAFQUAT HS-100, the average substance usage per site is expected to be 100 kg per annum.

The expected total polymer wastage factor will be 0.5% from unused residues in the polymer containers, equipment washings and batch residues. Given that a typical manufacturing plant will produce a batch of hair conditioner on 100 days of the year, the

expected daily waste polymer release will be 5g. Therefore, it is expected that approximately 500 g of polymer per site will be disposed of annually. These batch residues and polymer container residues will be disposed of to landfill while equipment washings will be processed through a treatment system for separation of solids and oils and precipitated into sludge. The dried sludge is expected to be disposed of to landfill.

GAFQUAT HS-100 is intended solely for use in hair care products and, as such, would be expected to be released to the environment via consumer use through washing the polymer from the hair into the sewerage system.

Due to the presence of quaternary ammonium groups in its structure, GAFQUAT HS-100 is likely to bind strongly to the sludge/solids compartment of the sewerage system where it is expected to be incinerated, disposed of to landfill or spread onto agricultural land.

. **Fate**

The notifier states that by nature of the application, the polymer is required to be stable under a wide range of conditions. The polymer will form water vapour and oxides of carbon and nitrogen on combustion.

GAFQUAT HS-100 is likely to persist in landfill situations given its relatively high adsorption coefficient and stated chemical stability.

9. **EVALUATION OF TOXICOLOGICAL DATA**

9.1 **Acute Toxicity**

Although toxicity information is not required for polymers with a NAMW > 1000 tests had been conducted on the notified substance in a 34% aqueous solution and these are summarised in table 1.

Table 1 Summary of the acute toxicity of Agent AT-1269 (34% aqueous solution)

Test	Species	Outcome	Reference
Acute Oral Toxicity	Rat	LD50 > 5 g/kg bw	1
Skin Irritation	Rabbit	Non-irritant	2
Eye Irritation	Rabbit	Minimally Irritating	3

9.1.1 Oral Toxicity (1)

Five male and five female Wistar rats were deprived of food but not water overnight prior to dosing. The test article at 5 g/kg body weight was administered by gavage. Following administration the animals were allowed food and water *ad libitum* for a 14 day observation period.

One female died on day 2 after exhibiting muzzle staining, yellow genital staining and signs of diarrhoea. Another female exhibited yellow anal-genital staining and signs of diarrhoea on day 3. The yellow staining is presumed to be due to the fact that that the substance administered was a yellow liquid.

No other deaths or signs of toxicity were noted. The LD50 was greater than 5 g/kg.

9.1.2 Skin Irritation (2)

A 0.5 ml portion of the test article was applied to one abraded and one intact test site on each of the backs of 6 New Zealand White rabbits. Gauze patches were placed over the treated areas and an occlusive dressing was wrapped around the trunks of the animals to hold the patches in place.

The wrapping was removed after 24 hours and the sites wiped free of the test article with deionised water. The treated areas were examined for erythema and oedema at 4, 24, 48 and 72 hours. No erythema or oedema was observed in the intact skin of any of the 6 rabbits at any time point. The test article was concluded to be non-irritating to rabbit skin.

9.1.3 Eye Irritation (3)

A 0.1 ml sample of the test article was instilled into the conjunctival sac of one eye of each of 6 New Zealand White rabbits and the lids held together for about 1 second to prevent loss of the article. The untreated eye served as control. Both the test and control eyes of 3 of the rabbits were washed after 30 seconds with tepid tap water (approximately 1 L/min) for 1 minute. The treated eyes were examined at 1 hour and 1, 2, 3, 4 and 7 days following instillation of the test article.

No iritis or corneal opacity was noted for any of the rabbits during the observation period.

Conjunctival irritation was observed for both washed and unwashed eyes. No conjunctival irritation was observed after day 2. It was concluded that the test article was minimally irritating for both washed and unwashed eyes. Average Draize scores of 13.3, 4.0 and 2.0 were observed for 1 hour, 1 day and 2 days post-treatment respectively. Rinsing of eyes was marginally palliative. The test article can be concluded to be minimally irritating to the rabbit eye.

9.2 Genotoxicity

9.2.1 Salmonella typhimurium Reverse Mutation Assay (4)

The mutagenicity of a 20% solution of Agent AT-1269 was tested in the Ames strains TA1535, TA1537, TA1538, TA98 and TA100 with and without metabolic activation provided by the addition of rat liver S9. Negative and positive controls gave the expected responses.

No induced mutants were observed at test article concentrations up to 10,000 µg per plate.

9.2.2 Micronucleus Assay in the Bone Marrow Cells of the Mouse (5)

The test article, a 20% aqueous solution of Agent AT-1269, was administered by gavage at 0, 500, 2500 and 5000 mg/kg body weight to 10 ICR mice per dose per kill time group. Animals were killed at 24, 48 and 72 hours for extraction of the bone marrow.

Agent AT-1269 did not induce a significant increase in micronuclei in bone marrow polychromatic erythrocytes. Positive and negative controls gave the expected responses.

9.3 Human Studies

9.3.1 Dermal Sensitisation (6)

Agent AT-1269 was tested for contact dermal sensitisation in 110 human subjects. The induction phase consisted of a series of 9 applications of 0.2 ml of a 5% solution of the test article over a 3 week period, applied under an adhesive patch to an area of the left upper back. Approximately 2 weeks after the end of the induction phase, subjects were challenged with a single application (0.2 ml, 5% solution) to a virgin area of the right upper back. Sensitisation was assessed 24 - 96 hours later.

A total of 104 subjects completed the test. No skin reactions were noted during the induction or challenge phases. Agent AT-1269 therefore lacked sensitisation potential under the conditions of the test.

9.3.2 Phototoxicity (7)

Agent AT-1269 (0.2 ml, 5% solution) was applied in adhesive patches to the forearms (volar surface) of each of 10 human subjects. After 24 hours contact, one arm of each subject was irradiated with UV-A (0.22 J/cm²/minute for 15 minutes). Reaction was assessed 24 and 48 hours later.

No reactions were observed at irradiated or unirradiated sites. Agent AT-1269 did not induce contact dermal phototoxic responses under the conditions of the test.

9.3.3 Photoallergy (8)

Agent AT-1269 was tested for contact dermal photoallergy in 29 human subjects. The induction phase consisted of a series of 6 applications of 0.2 ml of a 5% solution of Agent AT-1269 over a 3 week period, applied under adhesive patches on the volar surface of the forearm. Twenty four hours after each application, arms were irradiated with UV-A (3.33 J/cm²) and UV-B (dosage in the range 75 seconds at 90 mJ - 105 seconds at 126 mJ depending on previously assessed skin type). Untreated irradiated patches and treated non-irradiated patches were used as controls.

Approximately 2 weeks after the end of the induction phase, subjects were challenged with a single application (0.2 ml, 5% solution) followed by UV-A irradiation to a virgin area of the forearm. Skin reaction was assessed 24 and 48 hours after irradiation.

A total of 28 subjects completed the test. Minimal erythema or erythema and/or slight oedema were exhibited at the irradiated sites by 26 subjects during induction. Similar findings were recorded on untreated irradiated patches in 6 subjects. At the challenge phase, minimal erythema was noted on treated irradiated sites in 4 subjects. One subject showed similar findings on treated non-irradiated sites and no reactions were observed on untreated irradiated sites.

Slight irritation was evident on UV-A and UV-B irradiation of treated skin during the induction phase but Agent AT-1269 did not induce contact photoallergy in humans under the conditions of the test.

9.4 Overall Assessment of Toxicological Data

Agent AT-1269 as a 34% aqueous solution, was of very low acute oral toxicity, was non-irritating to rabbit skin and was minimally irritating to the rabbit eye.

Agent AT-1269 was not genotoxic as judged by negative responses in the Ames test and the mouse micronucleus assay.

In humans Agent AT-1269 was not a sensitiser, was not phototoxic and was not photoallergenic.

Overall the notified polymer is of low toxicity.

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

No ecotoxicological data were provided, which is acceptable for polymers of NAMW > 1000 according to the Act.

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

The polymer is unlikely to present a hazard to the environment at any stage of its use, whether it be when reformulated into

cosmetic products (resulting in an estimated 500 g.year⁻¹ per site of reformulation waste disposed of to landfill) or when consumers wash the polymer residue from their hair.

If the polymer remains suspended, a predicted environmental concentration (PEC) for the substance in sewage water throughout Australia can be estimated from the following assumptions: 1 tonne maximum annual use, an Australian population of 17 million and a daily per capita water usage volume of 150 L. This provides a PEC of 1 ppb in sewage water which would be swiftly reduced to insignificant levels (likely to be in the parts per trillion range) by precipitation or dilution in rivers, lakes and oceans which act as receiving waters to nearly all sewage treatment plants in Australia.

The notified substance is not expected to exhibit toxic characteristics because large polymers of this nature are not readily absorbed by biota.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

The notified polymer was of low acute toxicity and was not genotoxic in animal tests. In humans, the polymer was tested for sensitising, phototoxic and photoallergenic responses because of its intended use in hair conditioners. These tests were negative. As the exposure to the polymer in normal use is very low both in amount and in duration, the effects of repeated use are not expected to be great.

In the occupational setting, the high viscosity of GAFQUAT HS-100, which is used in the manufacturing process, suggests that inadvertant spillage would be an unlikely event during weighing and mixing operations. Although mixing involves relatively high temperatures (70°C) in open containers, aeration is avoided to achieve a good quality product and mists are unlikely to be produced. Thus, exposure during reformulation of the notified substance is expected to be low and occupational health and safety effects are expected to be minimal.

13. RECOMMENDATIONS

To minimise occupational exposure to Agent AT-1269 the following guidelines and precautions should be observed:

- . personal protection complying with Australian Standards should be worn, for example, impermeable gloves as described in AS 2161 (9) and protective clothing as described in AS 3765.1 and AS 3765.2 (10, 11);
- . good work practices should be implemented to avoid spillages and splashing;
- . good housekeeping and maintenance should be practised; spillages should be cleaned up promptly with absorbents which should then be put into containers for disposal in accordance with local or State regulations;
- . the workplace should be well ventilated;
- . good personal hygiene should be observed; and
- . a copy of the Material Safety Data sheet should be easily accessible to employees.

14. MATERIAL SAFETY DATA SHEET

The Material Safety Data Sheet (MSDS) for GAFQUAT HS-100 was provided in Worksafe Australia format (12).

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the *Industrial Chemicals (Notification and Assessment) Act 1989* (the Act), secondary notification of Agent AT-1269 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

1. GAF Chemicals Corporation, USA, Modified Agent AT-1269 (9406-107) (34% Solids) Acute Oral Toxicity, Single Level - Rats. Data on file, Project No.: 89-6764A, 1989.
2. GAF Chemicals Corporation, USA, Modified Agent AT-1269 (9406-107) (34% Solids) Primary Skin Irritation - Rabbits. Data on file, Project No.: 89-6764A, 1989.
3. GAF Chemicals Corporation, USA, Modified Agent AT-1269 (9406-107) (34% Solids) Primary Eye Irritation, 3 Unwashed and 3 Washed - Rabbits. Data on file, Project No.: 89-6764A, 1989.
4. GAF Chemicals Corporation, USA, Mutagenicity Test on Agent AT-1269 in the Ames Salmonella/Microsome Reverse Mutation Assay. Data on file, Project No.: 10608-0-401, 1989.
5. GAF Chemicals Corporation, USA, Mutagenicity Test on Agent AT-1269 (Formula #88156) in the *in vivo* Mouse Micronucleus Assay. Data on file, Project No.: 10608-0-455, 1989.
6. GAF Chemicals Corporation, USA, Test Material: Agent AT-1269, Repeated Insult Patch Test. Data on file, Project No.: 88-127, 1989.
7. GAF Chemicals Corporation, USA, Test Material: Agent AT-1269, Phototoxicity Test. Data on file, Project No.: 88-509T, 1989.
8. GAF Chemicals Corporation, USA, Test Material: Agent AT-1269, Photoallergy Test. Data on file, Project No.: 88-509A, 1989.
9. Australian Standard 2161-1978, "Industrial Safety Gloves and Mittens (excluding Electrical and Medical Gloves)", Standards Association of Australia Publ., Sydney, 1978.
10. Australian Standard 3765.1-1990, "Clothing for Protection Against Hazardous Chemicals, Part 1: Protection Against General or Specific Chemicals", Standards Association of Australia Publ., Sydney, 1990.

11. Australian Standard 3765.2-1990, "Clothing for Protection Against Hazardous Chemicals, Part 2: Limited Protection Against Specific Chemicals", Standards Association of Australia Publ., Sydney, 1990.
12. National Occupational Health and Safety Commission, *Guidance Note for the Completion of a Material Safety Data Sheet*, 2nd. edition, AGPS, Canberra, 1990.