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NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION AND ASSESSMENT SCHEME

FULL PUBLIC REPORT

PERFLUOROBUTANE

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Director
Chemicals Notification and Assessment

FULL PUBLIC REPORT

PERFLUOROBUTANE

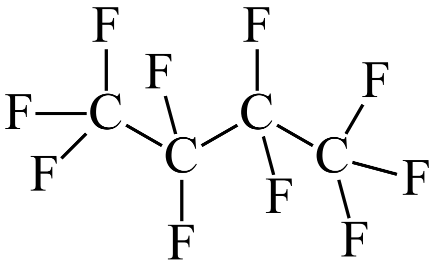
1. APPLICANT

3M Australia Pty Ltd of 2-74 Dunheved Circuit, St Marys, NSW 2760 has submitted a standard notification statement accompanying their application for an assessment certificate for perfluorobutane.

2. IDENTITY OF THE CHEMICAL

Chemical name:	Perfluoro-n-butane Decafluorobutane
Chemical Abstracts Service (CAS) Registry No.:	355-25-9
Other names:	L-12336 Lot 10 T-5411 F-10887 FC-3110
Trade names:	PFC-410 3M Brand Clean Extinguishing Agent CEA-410 3M Brand Clean Fire Extinguishing Agent PFG-5040 3M Brand Performance Fluid
Molecular formula:	$CF_3CF_2CF_2CF_3$

Structural formula:



Molecular weight: 238

Method of detection and determination:

The notified chemical can be isolated and determined by GC-MS, infrared and NMR spectral analysis.

Spectral data:

GC/MS analysis of L-12336 Lot 10 revealed that it contained 99.5% perfluorobutane (MW = 238), 0.34% tetrafluoropentene (MWt=142) and 0.02% of the sample was of unknown identity (MW = 132). Other smaller fractions were also identified.

IR	Major characteristic peaks were observed at 1313, 1258, 1238, 1152 and 901, 731 cm^{-1}, consistent with carbon-carbon stretching and carbon-fluorine stretching. Overall the spectrum is consistent with the structure of perfluorobutane.
NMR	A fluorine NMR spectrum was provided and was consistent with the expected structure of perfluorobutane. A proton NMR was also performed and revealed 0.004% hydrogen in incompletely fluorinated molecules.

3. PHYSICAL AND CHEMICAL PROPERTIES

Appearance at 20°C and 101.3 kPa:	colourless gas
Boiling Point:	-2°C
Melting Point:	-128°C
Gas Density:	9.935 kg/m^3 at 25°C and 1 atm
Vapour Pressure at 32°C:	3.26 atm
Water Solubility:	1.5 mg/L (at 1 atm perfluorobutane) by measurement of headspace pressure. The submission also includes a QSAR estimate of more than 100 mg/L. The solubility of the gas is estimated to be approximately 320 mg/L using Irmann's equation (1). The low measured solubility may reflect difficulties in retaining perfluorobutane in solution: the study reports a very low vapour to water partition coefficient of 0.00034 (nearly 3000 times as much perfluorobutane will exist in the vapour phase for equal volumes of vapour and water).
Partition Co-efficient (n-octanol/water) log P_{ow}:	> 3.93
Hydrolysis as a function of pH:	no functionalities normally considered to be hydrolysable
Adsorption/Desorption:	not applicable; significant sorption to soil is not expected as the notified substance is a gas
Dissociation Constant pK_a**:**	the notified chemical does not contain any readily dissociable groups
Flash Point:	not determined

Flammability Limits:	not applicable
Autoignition Temperature:	not determined
Explosive Properties:	not determined
Reactivity/Stability:	relatively inert

4. PURITY OF THE CHEMICAL

Degree of purity (percentage by weight):	> 99% C_4F_{10}
Toxic impurities:	none
Non-toxic impurities (> 1% by weight):	< 1% hydroperfluoroalkanes
Additives/Adjuvants:	none

5. INDUSTRIAL USE

Perfluorobutane will be used to replace Halon 1301 as a clean extinguishing agent for fire and explosion protection in certain applications involving public safety and national security that require a total flooding agent. Specific proposals are for telecommunications or computer equipment related to public safety and national security, life support function, and explosion suppression for flammable liquids and gases. Other uses may be military crewbays and confined spaces with difficult or impossible egress where second discharge may be required.

6. OCCUPATIONAL EXPOSURE

The notified chemical will be imported in cylinders containing up to 600 kg of gas at a rate of 1-10 tonnes/ year for the first 5 years.

Following transport by road to each of the 2 customer’s premises one storeman/ forklift driver is responsible for unloading the cylinders. The notified chemical is charged to smaller cylinders for use by fire system installers (plumbers and pipe-fitters). The charging operation involves purging the new cylinder with nitrogen followed by introduction of the notified chemical through a transfer pump. Progress of gas addition is measured by a weighing scale.

The configuration of valves and pipes is designed for the collection of both nitrogen and perfluorobutane that may be displaced during the filling operation and minimises unintended release into the workplace.

Fire system installation is expectd to follow design guidelines and methods accredited for use in the USA, a copy of which was provided by the notifier. The high cost of gaining independent accreditation in Australia is likely to preclude the use of alternative procedures. These procedures are stringent in identifying the correct hardware and design guidelines to be used and are expected to result in minimal unintended exposure to the notified chemical.

7. PUBLIC EXPOSURE

Public exposure to the notified chemical is expected to be low. The most likely exposure of the public to perfluorobutane is during discharge of extinguishers in the event of a fire, which does not occur very often. Exposure of this nature may result in inhalation, and ocular and dermal contact. It should be noted that the perfluorobutane acts to extinguish fire by eliminating oxygen, it thus has the potential to cause asphyxiation. This extinguishing agent is to be used in industrial, military, hospital and governmental establishments. The notified substance will not be sold direct to the public.

8. ENVIRONMENTAL EXPOSURE

Release

Repacking operations from larger to smaller containers, with possible addition of nitrogen to pressurise the receiving vessel, will occur at two locations. Minor leaks may escape to the atmosphere during these operations, for example when changing cylinders, but losses will be insignificant.

Environmental exposure to perfluorobutane will primarily occur through use of the agent. No additional training is required for use of the new agent, and no significant releases are expected, other than through use or system malfunction.

As part of its product stewardship program the notifier urges users to recover agent when testing, servicing or decommissioning fire protection systems, and recycle the agent for later use or destroy it. The notifier has indicated that material recovered will be returned to its US parent company for recycling. It is not expected that significant quantities of perfluorobutane will require disposal. Incineration, in the presence of combustible material, in an industrial or commercial facility equipped to handle gaseous waste, is recommended should local disposal be necessary.

Fate

Given its high volatility, any perfluorobutane released to the environment will partition rapidly and almost entirely to the atmosphere. Data provided by the notifier indicate that saturated solutions lose more than 90% of the perfluorobutane that they contain within 10 hours when stirred at ambient temperature in capped 40 mL vials containing 5 mL of solution. It is therefore inconceivable that aquatic organisms would be exposed for significant periods to perfluorobutane, and no bioconcentration is to be expected.

Any traces entering water would not be expected to undergo biodegradation at significant rates as degradation by activated sludge in a closed bottle test (OECD Test Guideline 301D) was minimal (28 d biological oxygen demand 12% of theoretical, with no degradation apparent from gas chromatography - reference 2).

The main degradation pathway in the environment is photochemical degradation upon exposure to short wavelength radiation (< 200 nm) in the upper stratosphere. As evidence exists for combustion in flames, thermal decomposition may also occur during passage through high temperature combustors such as power plants, incinerators and internal combustion engines (3). The estimated atmospheric lifetime is at least 2600 years.

Detailed atmospheric degradation pathways for perfluorobutane do not appear to have been elucidated. However, the applicant argues that no intermediate breakdown products will enter the biosphere as the onset of degradation will occur in the higher atmosphere, a high energy environment where breakdown products will not persist. This contrasts with HCFCs and HFCs used in fire protection, which degrade in the troposphere to a range of products including some, such as trifluoroacetate, that may persist in the environment.

It is unclear whether Australia has a disposal facility equipped to handle stable gaseous wastes of this nature at this time. However, significant quantities of waste requiring disposal are not expected. A plasma arc facility for destruction of halons is expected to become operational during 1996 and would represent an appropriate disposal option when available.

9. EVALUATION OF TOXICOLOGICAL DATA

For the inhalation toxicity studies with perfluorobutane, the atmosphere was not supplemented with oxygen. For the cardiac sensitsation study oxygen was maintained at 21% v/v at concentrations of perfluorobutane above 10% v/v.

9.1 Acute Toxicity

Summary of the acute toxicity of perfluorobutane

Test	Species (Strain)	Outcome	Reference
Inhalational toxicity	Rat (Sprague-Dawley)	No deaths, LD_{50} > 9.8% v/v in air or 79% v/v in oxygen	(4)
Cardiac sensitisation*	Dog (Beagle)	Non-sensitising	(5)

* cardiac arrhythmia (multiple multifocal ectopic heartbeats)

9.1.1 Inhalation Toxicity (4)

Sprague-Dawley rats (five/sex/group) were exposed (whole-body) for four hours to either an aerosol of 0 or 9.8% v/v perfluorobutane in air, or 79% v/v perfluorobutane in oxygen. Animals were observed for 14 days. No animals died during the study. No clinical signs of toxicity were noted in control or perfluorobutane/air-treated rats. During exposure the perfluorobutane/oxygen-treated rats had exaggerated respiratory movement. Males exposed to perfluorobutane displayed reduced weight gain. Food consumption was slightly lower for perfluorobutane rats on the day of exposure. The lung weight to bodyweight ratios were comparable. No treatment-related alterations to the lungs, liver or kidneys were noted.

9.1.2 Cardiac Sensitisation (5)

Ten male beagle dogs were used to study the cardiac sensitisation potential of perfluorobutane via inhalation (muzzle only). An intravenous injection of adrenaline was used before and during gas inhalation, and the effect of this injection was traced by electrocardiogram. The response of each dog to adrenaline (2-12 μg/kg) was studied using air in the inhalation chamber and appropriate doses of adrenaline were chosen for the main study. Trichlorofluoromethane (CFC 11), a known cardiac sensitiser as distinguished from an allergen, was used as a positive control. The following concentrations of perfluorobutane were used: 0, 5, 10, 20, 30 or 40% v/v in air.

Dogs exposed to 2% CFC 11 in air showed a positive cardiac sensitisation response. Dogs exposed to perfluorobutane did not show signs of cardiac sensitisation.

9.2 Repeated Dose Toxicity

9.2.1 Two-week inhalation (6)

Albino Sprague-Dawley CD rats (ten/sex/group) were exposed (whole-body) for two weeks (six hours per day, five days per week) to either 0 or 10% v/v perfluorobutane in air.

No deaths occurred in the study. No signs of clinical toxicity were observed. Slightly reduced bodyweight gain, food and water consumption were noted for females exposed to perfluorobutane. No differences in liver, kidney or lung weights were noted. Microscopic analysis of the kidneys, lungs, heart, liver and trachea did not reveal any treatment-related alterations.

9.2.2 Ninety-day inhalation (7)

Albino Sprague-Dawley CD rats (ten/sex/group) were exposed (whole-body) for 90 days (six hours per day, five days per week) to either 0, 0.5, 1.5 or 5% v/v perfluorobutane in air. A satellite group were exposed to either 0 or 5% v/v perfluorobutane in air for 90 days and observed for a further four weeks.

No deaths occurred in the study. No signs of clinical toxicity were observed. No changes in bodyweight gain or food consumption were noted. There were no treatment-related ophthalmological or biochemical changes. The following haematological parameters varied significantly for 5% treated rats; elevated mean corpuscular volume, notably higher total white cell and lymphocyte numbers for males, and reduced eosinophil numbers for females. No treatment-related pathological changes were noted. Ovarian weights for 1.5 and 5% rats were lower than controls. Ovarian weights were comparable for satellite groups.

9.3 Genotoxicity

Summary of genotoxicity studies

Test system	Species and strain	Test conditions	Results
Salmonella typhimurium, Reverse mutation assay	*S. typhimurium* (TA 1535, TA 1537, TA 1538, TA 100, TA 98)	5-80% v/v perfluorobutane in air ± ma*	Negative
Esherichia coli, Reverse mutation assay	*E. coli* (WP2 *uvrA*)	5-80% v/v perfluorobutane in air ± ma*	Negative
Chromosomal aberration assay	Chinese hamster lung cell line	10-80% v/v perfluorobutane in air ± ma*	Negative

* ma = metabolic activation

9.3.1 *Salmonella typhimurium* and *Escherichia coli* Reverse Mutation Assays (8)

Salmonella typhimurium, strains TA 98, TA 1537, TA 1538, TA 100 and TA 1535, and *Escherichia coli*, strain WP2 *uvrA*, were exposed to 5-80% v/v perfluorobutane in air. The plate incorporation technique was used both in the absence and presence of rat liver S9. The rat liver microsomal fraction (S9) was prepared from male Sprague-Dawley rats that had been treated with 500 mg/kg bw of Aroclor 1254. Air was used in the vapour phase as the negative control. Dimethylsulphoxide (DMSO) was used in the culture as the negative control. *N*-Ethyl-*N'*-nitro-*N*-nitrosoguanidine, 9-aminoacridine, 2-nitrofluorene and 2-aminoanthracene were used as positive controls.

Following exposure to perfluorobutane there were no increases in the number of revertant colonies in any of the six test strains used, either in the presence or absence of metabolic activation. The positive controls behaved as expected. Under the test conditions, perfluorobutane was not mutagenic in the *S. typhimurium* and *E. coli* reverse mutation assays.

9.3.2 *In vitro* chromosomal aberration assay (9)

Chinese hamster lung cells were exposed for six hours to 10-80% v/v perfluorobutane in air. These experiments were performed either in the presence of or absence of metabolic activation. Chromosomal preparations were prepared at six hours for metabolic activation and at 24 and 48 hours without metabolic activation. For metabolic activation, a microsomal liver fraction (S9) was prepared from male Sprague-Dawley rats that had been treated with 80 mg/kg β-naphthoflavone. Air was used in the vapour phase as the negative control. Methyl chloride and vinyl chloride were used as positive controls in the vapour phase. Mitomycin C and cyclophosphamide were used as positive controls in the culture medium.

Doses of up to 80% v/v perfluorobutane in air were not cytotoxic. There were no increases in the frequency of chromosomal aberrations in perfluorobutane treated cells. Elevated frequencies of chromosomal aberrations were found for the positive controls.

9.4 Overall Assessment of Toxicological Data

The acute inhalational toxicity of perfluorobutane in rats was low. Oral, dermal and eye irritation studies were not provided as these tests are not applicable to gases. Nevertheless, ophthalmoscopic observations performed during the 90 day chronic inhalation study did not provide evidence of eye irritation. During the inhalation studies the entire body of the rat was exposed to the notified substance. Perfluorobutane did not cause cardiac sensitisation. Rats repeatedly exposed to perfluorobutane for up to 90 days via the inhalational route showed only marginal effects on some white blood cell parameters. These effects were not consistent between the sexes. Perfluorobutane did not induce gene mutation in *Salmonella typhimurium* or *Escherichia coli*. There was no increased frequency of chromosomal aberrations *in vitro* in Chinese hamster lung cells exposed to perfluorobutane. Based on the studies presented perfluorobutane is not genotoxic.

Perfluorobutane would not be classified as hazardous according to Worksafe Australia's *Approved Criteria for Classifying Hazardous Substances* (10) in relation to Acute lethal effects (inhalation) or Severe effects after repeated or prolonged exposure (inhalational route).

10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

No specific data were provided, with the omission justified by the lack of significant aquatic exposure to this volatile and sparingly soluble gas. Perfluorocarbons are stable substances that do not exhibit significant biological activity, as exemplified by the results from testing on perfluorohexane. The nominal 96 hour LC_{50} for fathead minnow exposed under static conditions to this liquid perfluorocarbon (bp 56°C) exceeded the single dose tested of 1000 mg/L (11). The exact concentration to which fish were exposed is unclear as undissolved material remained at the bottom of the aquarium, but the perfluorocarbon clearly has no significant toxicity to fish.

Volatile halocarbons can affect the atmosphere. The principal concern is ozone depletion. Halon 1301 has a particularly high ozone depletion potential of 16 (12). Perfluorobutane contains neither chlorine nor bromine, and thus will not act as a source of ozone depleting halogen radicals in the stratosphere.

As with other halocarbons, perfluorobutane emissions will increase the global warming potential of the atmosphere. This would be of particular concern for the longer term if perfluorobutane were to be released in significant quantities, given the very long atmospheric lifetime. However, projected import volumes are relatively low and not expected to increase significantly as the high cost of the agent and the product stewardship measures in place are expected to restrict its use to specialised applications. Furthermore, radiative forcing is lower than might be anticipated as the infrared absorbances of perfluorocarbons occur at shorter wavelengths than for chlorofluorocarbons, in a spectral region in which less energy is radiated from the Earth because of attenuation by water and other trace gases. The notifer estimates a global warming potential of 5500 relative to carbon dioxide over a 100 year time horizon, intermediate between those for CFC-11 (3400) and CFC-12 (7100).

11. ASSESSMENT OF ENVIRONMENTAL HAZARD

Perfluorobutane is not expected to exert a direct effect on living organisms as it belongs to a class of compound, the perfluorocarbons, with negligible biological activity. The high volatility should ensure minimal exposure of aquatic and terrestrial compartments, and therefore minimal hazard to organisms inhabiting them.

Hazard to the atmosphere will be reduced when perfluorobutane replaces the strongly ozone depleting Halon 1301, as the replacement refrigerant has negligible potential to destroy ozone. However, the replacement retains significant global warming potential and is expected to persist in the atmosphere for millennia.

Because of the very high atmospheric persistence, perfluorobutane is considered to be an acceptable total flooding agent only in those limited instances where no other alternative is technically feasible due to performance or safety requirements. In most total flooding applications alternatives exist. The US EPA, for example, urges users not to select perfluorobutane out of simple preference, but out of need, and to use perfluorocarbons as the agents of last resort. The user is responsible for determining that the requirements of the specific end-use preclude utilization of other available alternatives and for keeping records of this determination.

The notifier operates a similar product stewardship program for local users, including provision of a decision tree to determine whether perfluorobutane is the correct agent for a given situation. Users must first determine whether a clean agent is required. If so, the questions of whether human exposure is likely and whether use of other clean agents may approach cardiosensitisation levels or be otherwise potentially injurious to health must be addressed. If so, perfluorobutane is the appropriate agent. If not, technical constraints of other agents (such as their physical and chemical properties) must still be considered to determine whether perfluorobutane is the appropriate agent.

The other main feature of the notifier's product stewardship operations is that unwanted perfluorobutane, including that recovered from equipment maintenance or decommissioning, will be returned to the US for recycling when no longer needed.

12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS

Perfluorobutane is expected to exhibit low acute and chronic inhalational toxicity and is not likely to be genotoxic. It is also not likely to exhibit cardiac sensitisation.

Exposure to perfluorobutane during repacking into smaller gas bottles and during fire system installation is expected to be minimal given the stringent procedures employed and the systems being designed to minimise unintended release.

Exposure to perfluorobutane is likely to be significant when there is a fire and total flooding occurs. As fires are expected to be infrequent events, exposure to perfluorobutane is expected to be low and the gas would be expected to disperse relatively rapidly after release.

The risk of adverse occupational and public health effects resulting from transport, storage, use and disposal of perfluorobutane is expected to be low given the low hazard and likely low or infrequent exposure. However, there is an occupational health risk of frostbite from exposure to sudden release of the compressed gas and there is a public health risk of asphyxiation if total flooding occurs in an enclosed area with limited means of egress.

13. RECOMMENDATIONS

To minimise occupational and environmental exposure to perfluorobutane the following guidelines and precautions should be observed:

- If engineering controls and work practices are insufficient to reduce exposure to perfluorobutane to a safe level, then personal protective devices which conform to and are used in accordance with Australian or Australian/New Zealand Standards (AS or AS/NZS) for respiratory protection (AS/NZS 1715, AS/NZS 1716) (13,14), eye protection (AS 1336, AS/NZS 1337) (15,16), impermeable gloves (AS 2161) (17) and protective clothing (AS 2919) (18) should be worn;

- Emissions of perfluorobutane should be minimised by only using the agent in accordance with the Code of Practice (19) for the Design, Installation, Inspection and Testing of Gaseous Fire Suppression Systems Utilising Ozone Depleting Substances (this requirement should appear on the Material Safety Data Sheet). Perfluorobutane should only be used where no alternative is technically feasible due to performance or safety requirements.

- Perfluorobutane should be recovered from maintenance and decommissioning of systems that contain it for recycling, storage or destruction; and

- The Material Safety Data Sheet (MSDS) should be updated when a plasma arc facility becomes available in Australia to indicate that this is the preferred method of disposal where recovery for recycling is not practical.

- A copy of the MSDS should be easily accessible to employees.

14. MATERIAL SAFETY DATA SHEET

The MSDS for perfluorobutane provided was in accordance with Worksafe Australia's *National Code of Practice for the Preparation of Material Safety Data Sheets* (20).

This MSDS was provided by 3M Australia Pty Ltd as part of their notification statement. The accuracy of this information remains the responsibility of 3M Australia Pty Ltd.

15. REQUIREMENTS FOR SECONDARY NOTIFICATION

Under the *Industrial Chemicals (Notification and Assessment) Act* 1989, secondary notification of perfluorobutane 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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