HPV Robust Summaries and Test Plan

CAS# 86508-42-l Perfluoro compounds, C5-C 18, including CAS#3 1 l-89-7 Perfluorotributyl amine

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1.0 Description of CAS number

1.1 Introduction

This HPV submission addresses a class of inert perfluorinated compounds (PFCs) covered by a single "generic" CAS# 86508-42- 1, defined as "Perfluoro-compounds, C5-C 18 ." (This "generic" CAS number is listed on the TSCA inventory based on the EPA's suggestion upon submittal of 3M's consolidated PMN 82-612 through 82-626.) Many compounds covered by this generic CAS number also have individual CAS numbers. However, only the generic CAS number and one individual CAS number (#3 1 l-89-7, perfluorotributyl amine) which is covered by the generic CAS number, are HPV chemicals based on the 1990 Inventory Use Reports used to designate HPV chemicals.

Data are available on a number of compounds within the generic CAS number for PFCs. This test plan presents existing data on ten different products that consist of various PFCs. It is well established that PFCs are chemically and biologically inert. Together the available data are ample to represent CAS # 86508-42-1, including CAS # 31 l-89-7, and no further testing is proposed.

PFCs are inert fluids composed of a complex combination of organic compounds resulting from the distillation of electrochemically fluorinated (ECF) compounds. This class consists of branched, linear and cyclic perfluorinated hydrocarbons having carbon numbers predominantly in the range of C5-C18 and boiling in the range of approximately 25° C to 255" C (77" F – 491" F). Perfluorinated amine and ether compounds may also be present.

3M manufactures a number of products comprised of PFCs, and markets them subject to rigorous product stewardship because of their photochemical stability and global warming potential. Section 1.2 lists ten products, each with its own individual CAS number, that are included under this "generic" CAS number and for which data are presented in this test plan. This listing is not intended to be inclusive of all possible chemicals covered by the generic CAS number. Rather, it represents the PFC products manufactured by 3M that were included in 3M's 1990 IUR submission. Data on these products adequately represent the generic CAS number.

CAS #3 1 l-89-7 is specifically identified in the title of this voluntary HPV submission because the EPA lists it as a separate HPV chemical. 3M did report this product separately in its 1990 IUR submission. However, CAS #3 1 l-89-7, like a number of other products with individual CAS numbers, is encompassed within the "generic" CAS number. It is included in this test plan, rather than separately, because it meets the toxicologic and environmental profile of this class of compounds. The term PFCs in this document encompasses CAS #3 1 l-89-7.

This test plan presents physical property data on each of ten PFC products. PFCs are highly volatile and insoluble in water. For the environmental and toxicological HPV endpoints, this test plan summarizes data from one or more PFC products. Data are available for almost all relevant endpoints, although certain physical property and environmental fate tests are not applicable. Ecotoxicity tests for fish and aquatic invertebrates show no toxicity; aquatic plant testing is deemed unnecessary. Acute toxicity, genotoxicity and repeat dose toxicity data are

available. Acute oral and inhalation toxicity tests show no toxicity at any dose tested, and even extremely high-dose intraperitoneal injection resulted in no lethality. Ames testing showed no genotoxicity. Inhalation exposure at levels up to 50,000 ppm for thirteen weeks produced no effects in rats, nor did oral exposure for thirty days at 2,000 mg/kg/day. Further testing for reproductive or developmental effects is unnecessary and inappropriate given that PFCs are chemically and biologically inert.

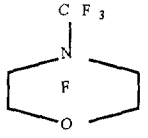
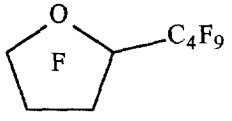
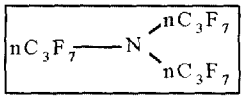
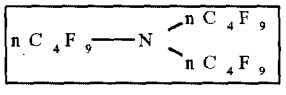
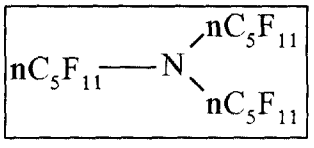
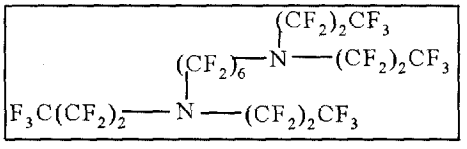
The compounds within this class of materials are all fully fluorinated and do not contain functional end-groups. As such, the materials within this class are all chemically and biologically inert. PFCs have high Henry's constants which dictate their environmental partitioning and, as described in Section 1.3, their low potential for interaction with biological membranes. The available data on this class of material demonstrates very consistent properties with regard to human health and environmental impact. The commonalities within this class are not surprising given the underlying physical/chemical properties.

The chemical and biological stability of this class of materials also results in very long atmospheric lifetimes. The persistence of these materials in the atmosphere and their global warming potential are the primary consideration for the strict product stewardship associated with the marketing and use of these materials. That stewardship dictates that this class of materials be used in niche applications where there are no other alternatives available on the basis of performance or safety.

1.2 Identity of Substances and Structural Classification

3M manufactures ten products that fall within the generic CAS # 86508-42- 1. As noted above, each of these products also has an individual CAS number, although EPA suggested use of the generic CAS number for inventory reporting.

The table below shows the composition of each PFC product, identifying the predominant molecule representing at least 50% of the total composition of the product as manufactured by 3M. The balance of each product is comprised of other PFCs with the same and similar number of carbon atoms in branched, linear and/or cyclic structure.

Product	CAS#	Predominant Molecule	Structural Formula
A	678-26-2	Perfluoropentane (C5)	$CF_3CF_2CF_2CF_2CF_3$
B	382-28-5	Perfluoro-N-methylmorpholine	
C	355-42-0	Perfluorohexane (C6)	$CF_3CF_2CF_2CF_2CF_2CF_3$
D	335-57-9	Perfluoroheptane (C7)	$CF_3CF_2CF_2CF_2CF_2CF_2CF_3$
E	307-34-6	Perfluorooctane and	$CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_3$
	335-36-4	Perfluoro-2-butyltetrahydrofuran (cyclic perfluoroether)	
F	307-34-6	Perflurooctane (C8)	$CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_3$
G	338-83-0	Perfluorotripropylamine	
H_a/H_b	311-89-7	Perfluorotributylamine	
I	338-84-1	Perfluorotriamylamine	
J	143356-32-5	Perfluoro-N,N,N',N'-tetrapropyl hexanediamine	

1.3 Summary of Chemical and Physical Properties and Lack of Ecological and Toxicological Effects

PFCs are among the least toxic of all known organic chemicals. PFCs don't oxidize or hydrolyze. They have no functional reactive groups. PFCs owe their low toxicity to the combination of the following properties:

1. Chemical inertness
2. Low solubility in biological media (blood, cell membranes, etc.)
3. High volatility
4. Resistance to biological activation (reductive and oxidative metabolism)

Because PFCs are chemically inert, if inhaled and absorbed they do not react chemically with any biological molecules; they simply partition between blood and various organs and tissues. As PFCs have limited ability to dissolve in biological media, they do not reach appreciable concentrations in the tissues of air-exposed animals. As PFCs are highly volatile chemicals and have high air-blood partition coefficients, any fluorochemical remaining after exposure will be rapidly eliminated in the breath. Consequently, all such PFCs have:

1. Very high rodent LC50s (very low acute toxicity)
2. Very high cardiac sensitization EC50s (very low toxicity)

In fact, most PFCs do not induce narcosis (sleep) or cardiac sensitization at maximum achievable concentration (saturation).

PFCs are neutral molecules and because they are maximally fluorinated, they cannot undergo biological oxidation-reduction reactions to form reactive aldehydes, acid fluorides, radicals or acids that have been associated with several types of toxicity. As PFCs are not reactive directly with biological tissue and PFCs cannot form reactive metabolites, these fluorochemicals have tested negative in bacterial mutagenicity assays. Since PFCs are volatile and have limited water solubility, they also have very low toxicity when tested in fish and daphnia studies. These PFCs do not present any significant hazard to aquatic life.

Consequently, all PFCs that have undergone evaluation by the ACGIH or WEEL committees in the US have been granted an exposure guideline of 1000 ppm 8-hour Time Weighted Average (8-hr TWA). NASA has evaluated the toxicity information associated with PFCs including those that can be used as heat transfer agents and fire extinguishing agents in spacecraft and has established a Space Maximum Allowable Concentration (SMAC) of 11,000 ppm for up to 180 days (24 hours/day). (Chiu-Wing Lam, NASA, reference).

1.4 Use Pattern

PFCs are characterized as very stable, non-toxic liquids that have a very high dielectric and very low solubility for water and other airborne contaminants. These materials are also very insoluble in water. In other words, water does not go into PFCs and PFCs do not go into water. These specialty chemicals are used primarily in the industrial electronics industry for applications that exploit these specific properties. The principal applications include industrial heat transfer in semiconductor processing, electronics testing and solvents for computer disc drive lubrication.

Most applications where PFCs are used are regulated by section 612 of the Clean Air Act, which addresses the acceptability of alternatives for ozone-depleting substances. Based on the long atmospheric lifetime and high global warming potential of this class of materials, EPA regulations specify that PFCs may only be used as replacements for ozone-depleting substances in the regulated sectors where they are the only alternative available on the basis of either performance or safety. 3M follows this same guidance in applying product stewardship principles for supply of PFCs to unregulated sectors.

3M has manufactured PFCs at three sites in the U.S. Process improvements have reduced emissions 40% since 1995. 3M anticipates that installation of abatement technology in the next 3 years will reduce emissions to the environment by approximately 90% compared to the 1995 baseline. Although end-use applications are tightly controlled, emissions to the environment do occur at a very low rate. When emitted during manufacturing or from industrial use, the high Henry's Constant for this class of materials dictates preferential partitioning to the atmosphere.

2.0 HPV Test Plan

This chart represents the HPV Test Plan for CAS # 86508-42-1, Perfluoro compounds, C5-C18, including CAS # 311-89-7. This test plan reflects extensive existing data included in this submission. 3M does not propose additional testing.

Endpoint	Information Available	Acceptable	Testing Needed
Physical Properties			
Melting Point	N/A	Yes	No
Boiling Point	Yes	Yes	No
Relative Density	Yes	Yes	No
Vapor Pressure	Yes	Yes	No
Octanol/Water Partition Coefficients	Yes	Yes	No
Water Solubility	Yes	Yes	No
pH and pKa Values	N/A		No
Oxidation/Reduction Potential	N/A		No
Adsorption/Desorption to Soil	N/A		No
Environmental Fate and Pathways			
Photodegredation	Yes	Yes	No
Stability in Water	N/A		No
Biodegredation	Yes	Yes	No
Fugacity	Yes	Yes	No
Ecotoxicity			
Acute Toxicity to Fish	Yes	Yes	No
Acute Toxicity to Aquatic Invertebrates	Yes	Yes	No
Acute Toxicity to Aquatic Plants	No		No
Human Health Toxicity			
Acute Toxicity	Yes	Yes	No
Primary Irritation	Yes	Yes	No
Genotoxicity			
Point Mutation	Yes	Yes	No
Chromosomal Aberration	No		No
Repeat dose Toxicity	Yes	Yes	No
Special Endpoints	Yes	Yes	No
Reproductive Toxicity	No		No
Development and Teratogenicity Toxicity	No		No