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ADVANCED AGENT PROGRAM
CUP-BURNER TESTING OF SELECTED TROPODEGRADABLE CANDIDATES

Joseph L. Lifke
Ted A. Moore
Robert E. Tapscott

NEW MEXICO ENGINEERING RESEARCH INSTITUTE
The University of New Mexico
Albuquerque, New Mexico 87131-1376

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ROBERT A. TETLA
Project Officer

EDGAR F. ALEXANDER
Chief, Air Base Technology Branch

RICHARD N. VICKERS
Chief, Infrastructure Technology Section

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JOSEPH L. LIFKE
TED A MOORE
ROBERT E TAPSCOTT

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
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The University of New Mexico
Albuquerque, New Mexico 87131-1376

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WL/FIVC
139 Barnes Drive, Suite 2
Tyndall AFB FL 32403-5323
POC: Dr Juan Vitali, WL/FIVCF
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The objective of the overall advanced agent program is to develop new, highly effective chemicals to replace Halon 1211 in military streaming applications. The portion of the work discussed in this document has, as an objective, an initial investigation of tropodegradable compounds as Halon 1211 replacements for streaming agents. This report documents the determination of cup-burner extinguishment values for selected compounds.

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ABBREVIATIONS AND ACRONYMS

AFB	Air Force Base
ANSI	American National Standards Institute
APT	Advanced Protection Technologies
ASHRAE	American Society of Heating, Refrigerating, and Air Conditioning Engineers
CFC	Chlorofluorocarbon
EC_C	Extinguishment Concentration of Candidate Agent
EC_R	Extinguishment Concentration of Reference Agent
FC	Perfluorocarbons
GVEf	Gas Volume Effectiveness
GVEq	Gas Volume Equivalent
HFE	Hydrofluoroether
ICI	Imperial Chemicals Industry
MW	Molecular Weight
NFPA	National Fire Protection Agency
NMERI	New Mexico Engineering Research Institute
PFC	Perfluorocarbons
SVEf	Storage Volume Effectiveness
SVEq	Storage Volume Equivalent
USAF	United States Air Force
WEq	Weight Equivalent

PREFACE

This report was prepared by the New Mexico Engineering Research Institute (NMERI), The University of New Mexico, Albuquerque, New Mexico, for the Infrastructure Technology Section of Wright Laboratories (WL/FIVCF), Tyndall Air Force Base, Florida, under Contract F08635-93-C-0073, NMERI Project Number 8-31882. This document provides one of the final reports for the Advanced Agent Program.

The project Start Date was 5 December 1994, and the End Date was 31 October 1995. The WL/FIVCF Project Officer was Robert A. Tetla and the NMERI Principal Investigator was Robert E. Tapscott.

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EXECUTIVE SUMMARY

A. OBJECTIVE

The objective of the overall advanced agent program is to develop new, highly effective chemicals to replace Halon 1211 in military streaming applications. The portion of the work discussed in this document has, as an objective, an initial investigation of tropodegradable compounds as Halon 1211 replacements for streaming agents. This report documents the determination of cup-burner extinguishment values for selected compounds.

B. BACKGROUND

The production of halons, used for fire and explosion protection, ended on 31 December 1993 in developed nations. Among the candidates being developed to replace halons are the tropodegradable compounds. This report describes results from cup-burner tests of selected tropodegradable compounds.

C. SCOPE

Work to develop advanced halon replacements was initiated in September 1993 under the Advanced Streaming Agent Testing Program. The objective of this program, which is now being continued under the Advanced Agent Program, is to develop new advanced chemical replacements for Halon 1211 in streaming applications. Tropodegradable compounds, the subject of this report, is one portion of the Advanced Agent Program. Some of these compounds were reported previously.*

D. RESULTS

Cup-burner extinguishment concentrations were obtained for selected tropodegradable compounds. Test descriptions and results are presented. Cup-burner results range from 1.9 percent for heptadecafluoro-1-iodooctane ($CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_2I$) to 9.6 percent for trifluoro(trifluoromethyl)oxirane. Most of the compounds had cup-burner values in the range of 1.9 to 4.5 percent.

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* Skaggs, S. R., Heinonen, E. W., Moore, T. A., and Kirst, J. A., *Low Ozone-Depleting Halocarbons as Total-Flooding Agents, Volume 2: Laboratory-Scale Fire Suppression and Explosion Prevention Testing*, EPA-6001R-95-150b, Global Emission and Control Division, Air and Energy Engineering Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina, September 1993.

E. CONCLUSIONS

Of the agents reported within this scope of work, heptadecafluoro-1-iodooctane ($CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_2I$), pentafluoroiodoethane (CF_3CF_2I), and octafluoro-1,4-diiodobutane ($CF_2ICF_2CF_2CF_2I$) have the lowest extinguishment concentrations by volume percent. The agents with the best weight equivalents (WEq) and storage volume equivalents (SVEq) in relation to Halon 1211 are 2-bromo-3,3,3-trifluoro-1-propene ($CH_2=CBrCF_3$), pentafluoroiodoethane (CF_3CF_2I), and trifluoroiodomethane (CF_3I). All three agents have better SVEqs, and two of the agents (pentafluoroiodoethane and 2-bromo-3,3,3-trifluoro-1-propene) have better WEqs. The remaining agents had significantly higher SVEqs (32 percent greater or more) and WEqs (33 percent greater or more).

F. RECOMMENDATIONS

Although no tropodegradable replacement with a toxicity as low as that of Halon 1301 or 1211 has yet been identified, the results look very promising. A number of these agents are expected to have zero or near zero ozone depletion potentials (ODP). For example, one agent, trifluoromethyliodide (CF_3I) is as effective as Halon 1301 and has an atmospheric lifetime of less than one day.* Much work remains to be done in this area, and lower toxicity tropodegradable agents could be found.

One group of tropodegradable chemicals not studied in this initial investigation are the polar-substituted compounds. These include compounds with carbonyl groups (ketones, aldehydes, esters, carboxylic acids), compounds with hydroxyl groups (alcohols), ethers (particularly HFE derivatives), and amines, amides, and morpholines. Studies of these compounds is strongly recommended.

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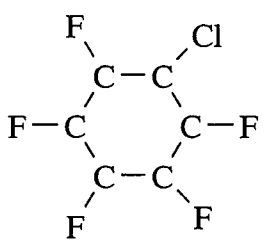
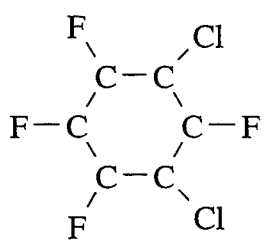
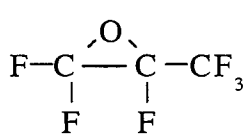
* Moore, T. A., Skaggs, S. R., Corbitt, M. R., Tapscott, R. E., Dierdorf, D. S., and Kibert, C. J., *The Development of CF_3I as a Halon Replacement*, Wright Laboratories, Tyndall Air Force Base, Florida, November, 1994. NMERI 1994/40 (Draft)

SECTION I
INTRODUCTION

Halon production ceased at the end of December 1993. A number of candidate replacement agents have been announced by industry for commercialization, and additional chemicals are under consideration. Work to develop advanced halon replacements was initiated in September 1993 under the Advanced Streaming Agent Testing Program. The objective of this program, which is now being continued under the Advanced Agent Program, is to develop new advanced chemical replacements for Halon 1211 in streaming applications. Tropodegradable compounds, the subject of this report, are one element of the Advanced Agent Program. Provided within this report are *n*-heptane cup-burner extinguishment concentrations for the tropodegradable compounds, and a discussion of the methods by which the agents were tested in the cup burner. Also discussed are the gas volume equivalents, the weight equivalents, and the storage volume equivalents for the various agents, with Halon 1211 as the reference compound. The tropodegradable agents that were tested in the cup burner are listed in Table 1. Material property sheets for the candidate agents are supplied in Appendix A.

Owing to long molecular chain lengths or to the presence of double bonds, the halocarbon numbers for several of these compounds are rather complex. For that reason, a discussion of the assignment of these numbers is presented in the following section.

TABLE 1. TROPODEGRADABLE COMPOUNDS TESTED IN THE CUP BURNER.

Halocarbon No.	Formula	IUPAC Name	CAS No.
13I1	CF_3I	Trifluoroiodomethane	2314-97-8
115I1	CF_3CF_2I	Pentafluoroiodoethane	354-64-3
217caI1	$CF_3CF_2CF_2I$	Heptafluoro-1-iodopropane	754-34-7
217baI1	CF_3CFICF_3	Heptafluoro-2-iodopropane	677-69-0
319I1	$CF_3CF_2CF_2CF_2I$	Nonafluoro-4-iodobutane	423-39-2
5-1-13I1	$CF_3CF_2CF_2CF_2CF_2CF_2I$	Tridecafluoro-1-iodohexane	355-43-1
7-1-17lI1	$CF_3CF_2CF_2CF_2CF_2CF_2$-CF_2CF_2I	Heptadecafluoro-8-iodooctane	507-63-1
318lccI2	$CF_2ICF_2CF_2CF_2I$	Octafluoro-1,4-diiodobutane	375-50-8
1233zdB1	$CHBr=CHCF_3$	1-Bromo-3,3,3-trifluoropropene	---
1233xfB1	$CH_2=CBrCF_3$	2-Bromo-3,3,3-trifluoropropene	1514-82-5
1242zfB1	$CH_2=CHCBrF_2$	3-Bromo-3,3-difluoropropene	420-90-6
1343fzbB1	$CH_2=CHCClFCBrF_2$	4-Bromo-3-chloro-3,4,4-trifluoro-1-butene	374-25-4
13441cczB1	$CH_2=CHCF_2CBrF_2$	4-Bromo-3,3,4,4-tetrafluoro-1-butene	18599-22-9
---		Chloropentafluorobenzene	344-07-0
---		1,3-Dichloro-2,4,5,6-tetrafluorobenzene	1198-61-4
---		Trifluoro(trifluoromethyl)oxirane	428-59-1

SECTION II
HALOCARBON NUMBERING SYSTEM

The "Halocarbon Numbering System" has become widely used, and an unofficial extended version has been used in both national and international regulations. The Halocarbon Numbering System (sometimes called the CFC, Freon®, or Refrigerant Numbering System) was developed by DuPont for Freon® chemicals in the late 1930s. The system was later expanded and formalized into a standard by the American Society of Heating, Refrigerating, and Air-Conditioning Engineers (ASHRAE) and the American National Standards Institute (ANSI) (Reference 1). Note, however, that this Standard uses the Halocarbon Numbering System only for derivatives of cyclobutane, propane, ethane, and methane. The unofficial, but widely used, extended numbering system described in the present report is applicable for larger molecules; however, this will give numbers that could conflict with refrigerant numbers assigned to other chemicals (particularly, blends or inorganics).

In the early days, many of the halocarbon chemicals used as refrigerants were given numbers preceded by the designation "Freon®"; however, since this is a trade name, other prefixes are now usually used. In the refrigeration industry, it is common practice to precede the halocarbon number with an "R"; however, such a prefix can be misleading for refrigerants other than butane, propane, ethane, or methane derivatives. A series of letters denoting the type of compound is now often used.* For example, compounds containing only chlorine and fluorine (in addition to carbon) have numbers preceded by "CFC" (chlorofluorocarbon). Though not universally accepted or standardized, other prefixes are being increasingly used. Table 2 lists the prefixes that have been adopted. Note that two prefixes are used for perfluorocarbons: "FC" and "PFC." Note also that this prefix nomenclature is beginning to be used for ethers. Thus "HFE" denotes a hydrofluoroether.

* The prefix has been omitted from the halocarbon numbers in Table 1 because the issue of whether such prefixes can be applied to unsaturated compounds (e.g., propenes and butenes) is unresolved.

In the Halocarbon Numbering System, the first number gives the number of carbon atoms minus one, followed by (in order) the number of hydrogen atoms plus one and the number of fluorine atoms:

first number	number of carbon atoms - 1
second number	number of hydrogen atoms + 1
third number	number of fluorine atoms

All remaining atoms are assumed to be chlorine atoms. An initial zero (indicating a one-carbon compound) is omitted. For example, CFC-12 has one carbon atom (the initial zero has been dropped), no hydrogen atoms (0 + 1 = 1), two fluorine atoms and, by default, two chlorine atoms, for a formula CF_2Cl_2. CFC-113 is CF_3CCl_3 or one of its isomers. When any number in the halocarbon designation contains two or more digits, dashes are used to separate the numbers. For example, $CF_3CF_2CF_2CF_2CClF_2$ is CFC-4-1-11 (ignoring isomer designations discussed below). It has been suggested that dashes be used only to set off the specific numbers with multiple digits, but this could be misleading. For example, CFC-41-11 could correspond to a 5-carbon compound or a 42-carbon compound (admittedly, unlikely).

TABLE 2. PREFIXES FOR HALOCARBON NUMBERS.

Prefix	Elements in Chemical	Chemical Family
BC	Br, C	Bromocarbon
BCC	Br, Cl, C	Bromochlorocarbon
BCIC	Br, Cl, I, C	Bromochloroiodocarbon
BCFC	Br, Cl, F, C	Bromochlorofluorocarbon
BCFIC	Br, Cl, F, Cl, C	Bromochlorofluoroiodocarbon
BFC	Br, F, C	Bromofluorocarbon
BFIC	Br, F, I, C	Bromofluoroiodocarbon
BIC	Br, I, C	Bromoiodocarbon
CC	Cl, C	Chlorocarbon
CFC	Cl, F, C	Chlorofluorocarbon
CFIC	Cl, F, I, C	Chlorofluoroiodocarbon
CIC	Cl, I, C	Chloroiodocarbon
FC	F, C	(Per)fluorocarbon
FE	F, C, O	(Per)fluoroether
FIC	F, I, C	Fluoroiodocarbon
HBC	H, Br, C	Hydrobromocarbon
HBCC	H, Br, Cl, C	Hydrobromochlorocarbon
HBCFC	H, Br, Cl, F, C	Hydrobromochlorofluorocarbon
HBCFIC	H, Br, Cl, F, I, C	Hydrobromochlorofluoroiodocarbon
HBCIC	H, Br, Cl, I, C	Hydrobromochloroiodocarbon
HBFC	H, Br, F, C	Hydrobromofluorocarbon
HBFIC	H, Br, F, I, C	Hydrobromofluoroiodocarbon
HBIC	H, Br, I, C	Hydrobromoiodocarbon
HC	H, C	Hydrocarbon
HCC	H, Cl, C	Hydrochlorocarbon
HCFC	H, Cl, F, C	Hydrochlorofluorocarbon
HCFIC	H, Cl, F, I, C	Hydrochlorofluoroiodocarbon
HCIC	H, Cl, I, C	Hydrochloroiodocarbon
HFC	H, F, C	Hydrofluorocarbon
HFIC	H, F, I, C	Hydrofluoroiodocarbon
HFE	H, F, C, O	Hydrofluoroether
HIC	H, I, C	Hydroiodocarbon
IC	I, C	Iodocarbon
PFC	F, C	Perfluorocarbon
PFE	F, C, O	Perfluoroether

For cyclic compounds, the prefix "C" precedes the halocarbon number. For example, perfluorocyclobutane (cyclo-C_4F_8) is FC-C318. For unsaturated compounds, a number giving the number of double bonds is added on the left. Thus CF_2=CClF is CFC-1113. The presence of four numbers (may be more than four digits) always denotes an unsaturated compound.

A. TWO-CARBON COMPOUNDS (ETHANE AND ETHENE DERIVATIVES)

When there are two (or more) carbon atoms present, isomers are possible, and these may have identical halocarbon numbers. To distinguish these isomers for ethane derivatives, a lower case letter is added based on the difference in the sum of the atomic masses of the carbon substituents. The designation for the isomer with the smallest difference in the sum of the masses on the two carbon atoms has no letter; the designation corresponding to the next smallest difference has an "a", the next a "b", etc. Some examples are given below for the isomers of dichlorodifluoroethane.

$CHClFCHClF$	HCFC-132
$CHCl_2CHF_2$	HCFC-132a
$CClF_2CH_2Cl$	HCFC-132b
CCl_2FCH_2F	HCFC-132c

If bromine is present in the molecule, the halocarbon number is first assigned as if the bromine atoms were chlorine atoms (i.e., the halocarbon number is assigned for the "parent" molecule). The designation "Bn," where "n" is the number of bromine atoms, is then added to the end of the halocarbon number. For example, the anesthetic Halothane ($CF_3CHBrCl$) is HBCFC-123B1. The absence of a small letter indicates that this is the most symmetrical isomer, and the final "B1" means that one of the chlorine atoms was replaced with a bromine. The parent compound in this case is CF_3CHCl_2 (HCFC-123). As another example, $CClF_2CHBrF$, parent compound $CClF_2CHClF$, is HBCFC-123aB1 (omitting a final suffix for the bromine position, which is discussed below). CGET/NMERI has extended this further to include iodine compounds using a suffix "In," where "n" is the number of iodine atoms. This extension gives FIC-12I2 for CF_2I_2 and BFIC-12B1I1 for CF_2BrI.

Where the positions of the bromine atoms are ambiguous, Greek letter suffixes are added. The letters "α," and "β" denote the carbon atoms in the chain starting from the end carbon having the highest sum of atomic weights in the parent compound. HBCFC-123aB1 exists as two isomers — HBCFC-123aB1α ($CBrF_2CHClF$) and HBCFC-123aB1β ($CClF_2CHBrF$). Similarly, $CBrClFCBrF_2$ is HBCFC-113B2$\alpha\beta$ and CBr_2FCClF_2 is HBCFC-113B2$\alpha\alpha$.

NMERI/CGET has extended this to iodine-containing compounds: $CF_2ICHClF$ is HCFIC-123aI1α, $CClF_2CHFI$ is HCFIC-123aI1ß, $CClFICF_2I$ is CFIC-113I2αß, and CFI_2CClF_2 is CFIC-113I2αα. Where both bromine and iodine are present, the Greek letter position designations are placed after the appropriate designations giving the number of bromine and iodine atoms. For example, $CClFICBrF_2$ is BCFIC-113B1ßI1α and $CBrClFCIF_2$ is BCFIC-113B1αI1ß.

B. THREE-CARBON COMPOUNDS (PROPANE AND PROPENE DERIVATIVES)

The Halocarbon Numbering System for three-carbon compounds (propanes) is similar to that for two-carbon compounds; however, two letters are required to specify the isomer. (Letters are omitted when there is no possibility of isomerism.) The first letter refers to the central (methylene) carbon atom of the propane. To assign this letter, one calculates the combined atomic mass of the substituents on this carbon atom in the parent compound (containing only H, F, and/or Cl). The letter "a" represents the largest mass possible, the letter "b," the next largest, etc. The letters are assigned as shown in Table 3.

TABLE 3. METHYLENE CARBON DESIGNATIONS.

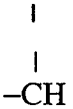
Suffix	Chemical Group
a	$-CCl_2-$
b	-CClF-
c	$-CF_2-$
d	-CHCl-
e	-CHF-
f	$-CH_2-$

The second letter is determined by the difference in the combined atomic masses of the substituents on the two terminal carbon atoms. The smallest difference is assigned the letter "a," the next smallest difference is assigned the letter "b," followed by "c," "d," etc. This method of isomer designation differs from that for two-carbon compounds, in which the smallest difference has no letter. For example, $CHCl_2CF_2CF_3$ (3,3-dichloro-1,1,1,2,2-pentafluoropropane) is designated HCFC-225ca, and the isomer $CHClFCF_2CClF_2$ (1,3-dichloro-1,1,2,2,3-pentafluoropropane) is HCFC-225cb.

If a three-carbon compound contains bromine or iodine, the suffix "Bn" or "In" is added as done for methane and ethane derivatives. Where the position of the bromine atom is ambiguous, Greek letter suffixes are again added. The letters "α," "β," and "γ" denote the carbon atoms in the chain starting from the end carbon having the highest sum of atomic weights in the parent compound. Thus, $CF_3CBrClCH_2Br$ (parent compound, $CF_3CCl_2CH_2Cl$) is HBCFC-233abB2βγ and $CF_3CHClCHI_2$ (parent compound $CF_3CHClCHCl_2$) is HBCFC-233daI2 αα. Application to mixed bromine/iodine derivatives is obvious: $CF_3CFBrCF_2I$ is BFIC-216baB1ßI1α, $CF_3CFICBrF_2$ is BFIC-216baB1αI1ß, and $CF_3CBrICF_3$ is BFIC-216aaB1I1. Note that the last compound is not designated as BFIC-216aaB1ßI1ß since the iodine and bromine must reside on the central atom for a compound with the Halocarbon Number 216aa. Isomer designation letters for both the parent compound and for the bromine or iodine positions are always omitted when no ambiguity can result.

Halocarbon designations for propenes contain four numbers starting with 1 (one double bond) and two lowercase letter suffixes. The first suffix designates the single atom attached to the central atom in the methine group (Table 4). The second letter gives the substitution on the terminal methylene carbon atom using the same letter designations as used for the central methylene carbon on propane derivatives (Table 3). Thus, $CH_2=CHCF_2Cl$ is HCFC-1242zf. Bromo- and iodopropenes are designated in the same way as for bromo- and iodopropanes and bromo- and iodoethanes (i.e., with suffixes "Bn" and "In"). Greek letters are added where necessary starting with the methylene end. Thus $CHBr=CBrCF_2Cl$ (parent compound, $CH_2=CClCF_2Cl$) is HCFIC-1232zfB2 (no Greek Letter descriptor is needed since the positions of the bromine atoms are fixed by the halocarbon number), and CHI=CBrCF2Cl is HCFIC-1232zfB1βI1α.

TABLE 4. METHINE CARBON DESIGNATIONS.

Suffix	Chemical Group
x	
y	
z	

C. COMPOUNDS WITH FOUR OR MORE CARBON ATOMS

Compounds with four or more carbon atoms are coded in a way similar to that used for compounds with fewer carbon atoms. To differentiate between isomers, carbon atoms containing a single substituent (methine carbons) are designated as shown in Table 4, carbon atoms with two substituents (methylene carbons) as shown in Table 3, and methyl groups as in Table 5. Letter designations begin at one end of the molecule (chosen to keep the alphabetical sequence as low as possible) for linear compounds. Bromine- and/or iodine-substituted compounds are handled in a fashion similar to that used for compounds with three or fewer carbon atoms.

TABLE 5. METHYL GROUP DESIGNATIONS.

Suffix	Chemical Group
j	$-CCl_3$
k	$-CCl_2F$
l	$-CClF_2$
m	$-CF_3$
n	$-CHCl_2$
o	$-CH_2Cl$
p	$-CHF_2$
q	$-CH_2F$
r	-CHClF
s	$-CH_3$
t	–C

Some examples for larger molecules are shown in Table 6. Note again that isomer designation letters not needed to describe a structure are omitted. Thus, $CCl_3CCl_2CCl_2CCl_2CCl_3$ is designated as CC-410 and not as CC-410jaaaj. Similarly, $CCl_3CF_2CF_2CF_2CF_3$ is CFC-4-1-9j; no additional letters are needed to describe the structure.

TABLE 6. EXAMPLES FOR COMPOUNDS WITH FOUR OR MORE CARBON ATOMS.

Compound	Halocarbon Number
$CCl_3CCl_2CCl_2CCl_2CCl_3$	CC-410
$CCl_3CF_2CF_2CF_2CF_3$	CFC-4-1-9j
$CF_3CClFCH_2CH_2F$	HCFC-355mb
$CF_3CBrFCH_2CH_2F$	HBFC-355mbfB1
$CF_3CHFCHFCF_2CF_3$	HFC-4-3-10mee
$CF_3CF_2CH_2CH_2F$	HFC-356mcf

D. ETHERS

Rules have been proposed for numbering ether-based refrigerants (Reference 2). Usually ether designations have an "E" or "CE" (in the case of cyclic ethers) immediately preceding the number; however, to avoid redundancy, the E immediately preceding the number is omitted here. For dimethylether derivatives, designation numbers are derived in the same way as those for the haloethanes. For straight-chain, three-carbon derivatives, the carbon atoms are numbered sequentially with "1" assigned to the end carbon with the least number of halogen atoms. When the end carbon atoms contain the same number of halogen atoms, number 1 is assigned to the end carbon having the largest number of iodine, then bromine, then chlorine, and finally fluorine atoms. The number giving the location of the ether oxygen is placed at the end of the suffix letters, which are retained when a single isomer exists. Some examples follow: $CF_3OCF_2CF_3$, FE-218ca1; $CHF_2OCHClCHF_2$, HCFE-244da1; and $CF_3OCH_2CHF_2$, HFE-245fa2. We can modify the proposed rules to include molecules containing four or more carbon atoms by using the method shown in the previous section, but starting with the end carbon containing the least number of halogen atoms. For example, $CF_3CF_2CF_2CF_2OCH_3$ is HFE-449s1 and $CF_3CF_2CF_2CF_2OCH_2CH_3$ is HFE-569sf2. Nomenclature rules have been proposed for only 3-carbon cyclic ethers. For such compounds, the oxygen atom is taken to be positioned between C1 and C3. Thus, $-CF_2CHFCF_2O-$ is HFE-CE225ea.

SECTION III
TROPODEGRADABLE COMPOUNDS

Tropodegradable replacements are halocarbons that have very low atmospheric lifetimes, leading, in most cases, to near-zero global warming and ozone depletion. There are two caveats. First, all compounds that are rapidly removed from the troposphere are designated "tropodegradable," whether or not the removal actually involves molecular destruction. Second, rapid removal is required for the use of this designation. Thus, although HCFCs and HFCs break down in the atmosphere, the breakdown is relatively inefficient, and these compounds are not considered tropodegradable. No sharp dividing line between rapid and non-rapid tropospheric degradation has been set; however, chemicals with atmospheric lifetimes of less than one year are proposed here as being tropodegradable.

Owing to their short atmospheric lifetimes, tropodegradable compounds have decreased global environmental impacts — global warming, potential for ozone depletion, and atmospheric persistence. At least five mechanisms (Table 7) are available to reduce the atmospheric lifetimes of molecules: (1) reaction with hydroxyl free radicals (OH), (2) photodecomposition, (3) rainout, (4) thermal decomposition, or (5) hydrolysis due to atmospheric moisture (Reference 3). Hydrolysis is generally unimportant here, however, since compounds that hydrolyze rapidly (e.g., compounds with halides) are usually toxic. For effective chemical suppression by halocarbons, bromine (or iodine) should be present. Tropodegradable bromocarbons may give global environmental acceptability.

TABLE 7. MECHANISMS FOR TROPOSPHERIC REMOVAL.

Primary Removal Mechanisms	Example Families	Specific Agents
Photodegradation	Iodides, aromatics	Perfluoroalkyl iodides, halobenzenes
Reaction with atmospheric hydroxyl	Unsaturated compounds (alkenes and, possibly, aromatics)	Bromoalkenes
Rainout	Polar substituted compounds (esters, ketones, alcohols, and, possibly, some ethers, amines, and amides)	Brominated alcohols, brominated ketones
Thermal decomposition	Epoxy compounds	Halogenated oxiranes
Hydrolysis	Compounds with halogens directly bonded to phosphorus, silicon, and metals	Halosilanes, halophosphines

A. IODIDES

Iodides photolyze readily giving extremely short atmospheric lifetimes. The atmospheric chemistry of iodides has been reviewed (Reference 4). Trifluoromethyl iodide, which is as effective as Halon 1301, has an atmospheric lifetime of less than one day (Reference 5). A number of studies have proposed and/or tested fluoroiodides as halon replacements (References 6 through 10).

Nine fluoroiodocarbons were evaluated in this study (Table 8). All the fluoroiodides tested have linear molecules, and all except $CF_2ICF_2CF_2CF_2I$ contain a single iodide atom.

TABLE 8. IODIDES.

Formula	IUPAC Name
CF_3I	Trifluoroiodomethane
CF_3CF_2I	Pentafluoroiodoethane
$CF_3CF_2CF_2I$	Heptafluoro-1-iodopropane
CF_3CFICF_3	Heptafluoro-2-iodopropane
$CF_3CF_2CF_2CF_2I$	Nonafluoro-4-iodobutane
$CF_3CF_2CF_2CF_2CF_2CF_2I$	Tridecafluoro-1-iodohexane
$CF_3CF_2CF_2CF_2CF_2CF_2$-CF_2CF_2I	Heptadecafluoro-8-iodooctane
$CF_2ICF_2CF_2CF_2I$	Octafluoro-1,4-diiodobutane

B. ALKENES

Alkenes are rapidly destroyed by hydroxyl free radicals in the troposphere giving atmospheric lifetimes on the order of days. Alkenes tend to be toxic; however, toxicity is reduced if the halogen atoms are kept away from the double bonds. Carcinogenicity and mutagenicity are of concern when the halogens are in the α and β positions.

Hexafluoropropene (Reference 11), *cis*- and *trans*-1,2-dichloroethenes (Reference 12), *n*-perfluorobutylethene (Reference 13), and hexabromo-2-butene (References 14 and 15), and bromoalkenes in general (References 16 and 17) have been proposed for use in fire suppressants and fire resistant treatments.

As noted above, in order to have a good fire suppressant capability, bromine (or iodine) should be present. Three bromopropenes and two bromobutenes were examined in the present study (Table 9).

TABLE 9. BROMOALKENES.

Formula	IUPAC Name
$CHBr=CHCF_3$	1-Bromo-3,3,3-trifluoropropene
$CH_2=CBrCF_3$	2-Bromo-3,3,3-trifluoropropene
$CH_2=CHCBrF_2$	3-Bromo-3,3-difluoropropene
$CH_2=CHCClFCBrF_2$	4-Bromo-3-chloro-3,4,4-trifluoro-1-butene
$CH_2=CHCF_2CBrF_2$	4-Bromo-3,3,4,4-tetrafluoro-1-butene

C. AROMATICS

There is relatively little information available on degradation of aromatics in the troposphere. Like the alkenes, the aromatics contain unsaturated bonds and may react with hydroxyl free radicals in the atmosphere. They are, however, considerably less reactive and, because of this lower reactivity, may have unacceptable atmospheric lifetimes. Aromatic compounds will also photolyze more easily than alkanes.

Ideally, brominated aromatics should be used to give enhanced fire suppression characteristics; however, in this initial brief investigation on chloro derivatives — chloropentafluorobenzene (C_6ClF_5) and 1,3-Dichloro-2,4,5,6-tetrafluorobenzene ($C_6Cl_2F_4$) — were tested.

D. REACTIVE MOLECULES

Highly reactive molecules can be removed from the atmosphere by multiple reaction mechanisms including thermodecomposition. One example of such compounds are the oxiranes, which contain the highly reactive, cyclic epoxy group. Trifluoro(trifluoromethyl)oxirane, C_3F_6O was a member of this group tested in the cup burner.

SECTION IV
CUP-BURNER EXTINGUISHMENT CONCENTRATIONS

A. CUP-BURNER TEST METHOD

One of the most widely used apparatuses for determining the fire extinguishment concentration of Halon 1301 and 1211 replacements is the cup burner. Originally developed by Imperial Chemical Industries (ICI) in 1970 and refined in 1973, the cup burner is the standard flame extinguishment test technique accepted by the NFPA. The cup-burner apparatus was developed to measure the vapor phase performance of a chemical as a fire suppressant. Volumetric air and agent flow rates are used to calculate the molar percent concentration of agent required for flame extinguishment. Different techniques and equipment setups are required for testing gaseous, liquid, and "highly-volatile" liquid agents (References 18 and 19). The cup-burner apparatus consists of a glass chimney containing a small glass flame cup filled with a liquid fuel or containing a central burner for a gaseous fuel. Measured amounts of extinguishing agent and air enter the bottom of the chimney, are mixed, and allowed to pass by the ignited fuel. The amount of extinguishing agent is increased until the flame is extinguished, and the percent (molar, gas volume) concentration of agent is calculated. This calculated value is called the cup-burner extinguishment concentration.

1. Gaseous Agent Cup-burner Test Method

Under previous USAF contracts, NMERI developed and refined a unique cup burner and several test methods. A different test method is used depending upon the characteristics of the agent being tested. The classical gaseous agent cup-burner test setup consists of monitoring the gaseous flow rate of the agent using a flow rotameter and a soap-film bubble meter, as shown in Figure 1.

2. Liquid Agent-Cylinder (Discharge) Cup-Burner Test Method

Recently, a unique test method was developed based upon a discharge cylinder, needle valve, and electronic scale with computer data acquisition (Figure 2). Liquid compounds and those with boiling points near room temperature are usually tested using the liquid agent-cylinder (discharge) cup-burner method. The average results from five tests are used to determine the extinguishment concentration of the compound being tested.

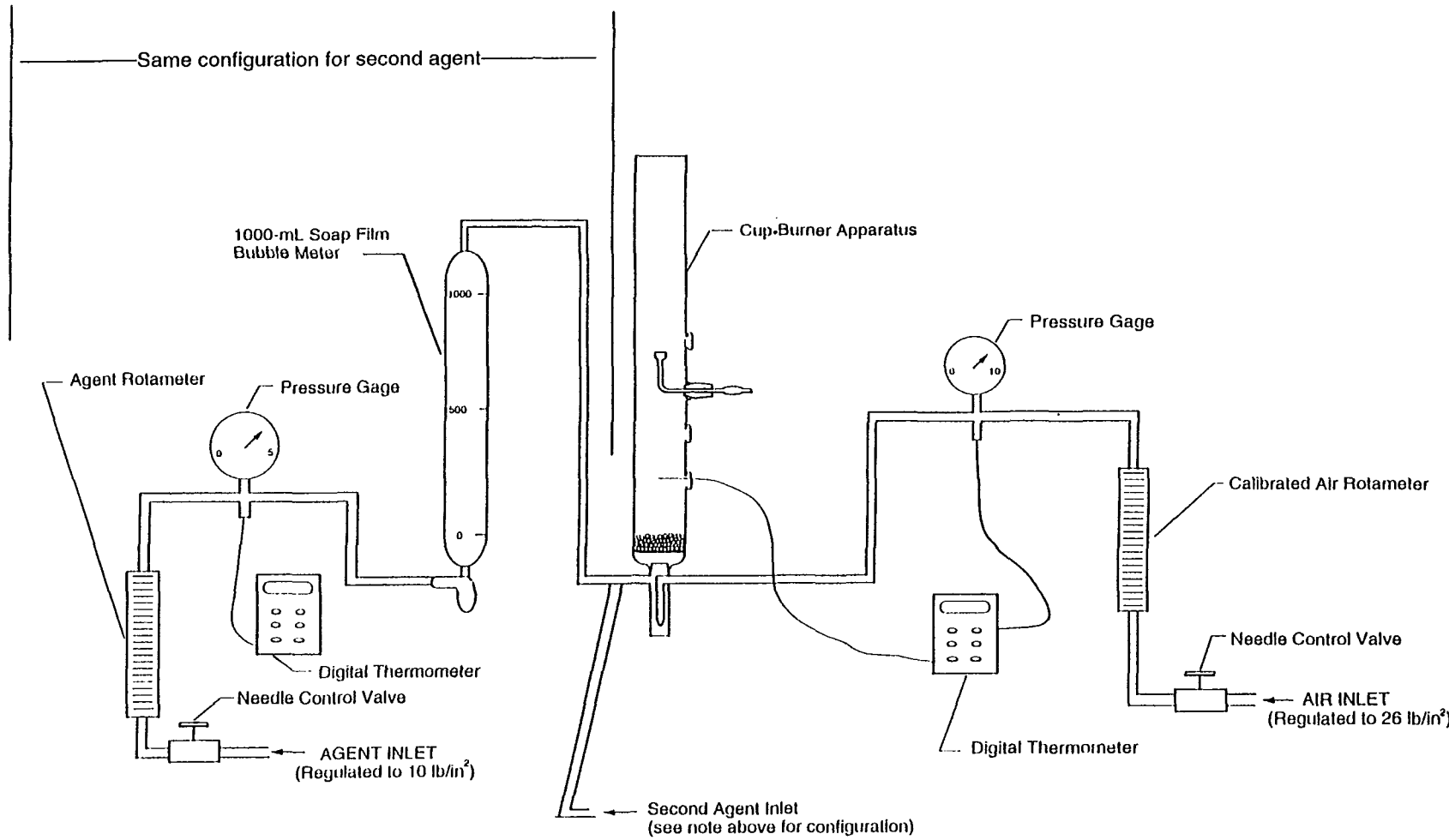


Figure 1. Cup-Burner Apparatus Configuration for Testing Gaseous Agents.

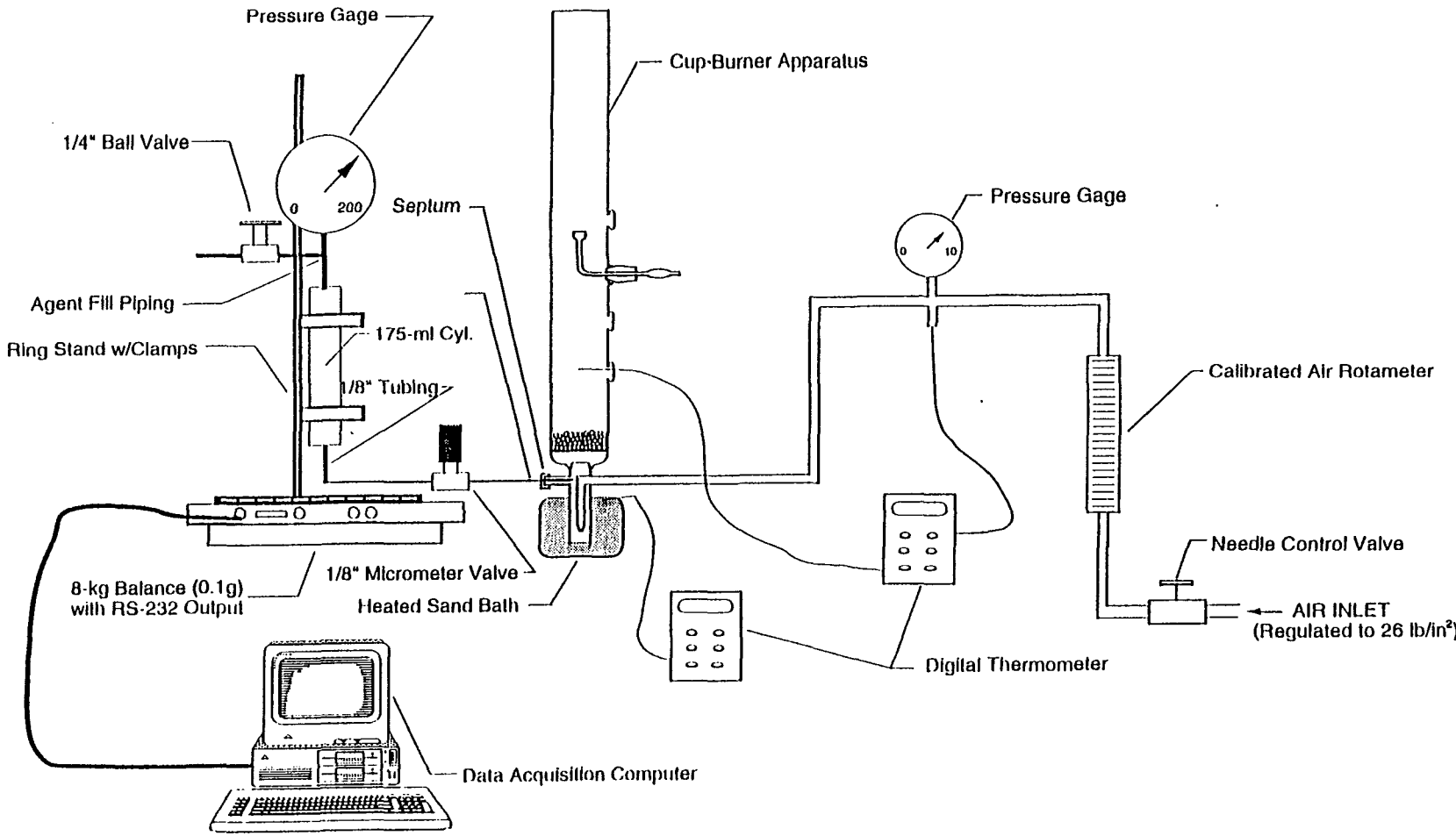


Figure 2. Cup-Burner Apparatus Configuration for Testing Liquid Agents.

B. DATA REDUCTION AND EXTINGUISHMENT TEST RESULTS

Extinguishment concentrations of gaseous agents are reported as volume percent concentration and are listed in Table 10. The molar flow rates for the air and gaseous chemicals were calculated using the ideal gas law and solving for n:

$$n = PV/RT \tag{1}$$

where

n = molar flow rate (moles/min)
P = atmospheric pressure (atm)
V = volumetric flow rate (mL/min)
R = gas constant (82.06 mL-atm/mole-K)
T = gas temperature in the chimney (K)

Once molar flow rates were determined, the extinguishment concentration, in percent, was calculated using the following equation:

$$EC = n_{agent}/(n_{agent} + n_{air}) \times 100 \tag{2}$$

where

EC = extinguishment concentration (%)

$$n_{agent} = P\ V_{agent}/R\ T \tag{3}$$

$$n_{air} = P\ V_{air}/R\ T \tag{4}$$

and

V_{agent} = agent volumetric flow rate (mL/min)
V_{air} = air volumetric flow rate (mL/min)

Substituting Equations (3) and (4) into Equation (2) gives the molar percent extinguishment concentration for gaseous agents as a function of the volumetric flow rates:

$$EC = V_{agent}/(V_{agent} + V_{air}) \times 100 \tag{5}$$

Based on analysis, the measurements of temperature and pressure within the cup-burner apparatus are unnecessary for determining gaseous agent extinguishment concentrations. These parameters fall out of the equation when the substitutions are made into Equation (2). Accurate air and agent volumetric flow rate measurements are the critical values in determining extinguishment concentrations.

The extinguishment concentration of liquid agents is calculated somewhat differently than that for gaseous agents because the flow rates are monitored differently. While the flow rates of gaseous agents are measured using calibrated rotameters, a discharge cylinder, needle valve, and electronic scale with computer data acquisition are used for the liquid agents. Therefore, the molar flow rates are calculated for liquid agents using the following equation:

$$n_{liq\ agent} = V_{liq\ agent}\, \rho / MW_{liq\ agent} \tag{6}$$

where

$n_{liq\ agent}$ = molar flow rate of the liquid agent (moles/min)
$V_{liq\ agent}$ = volumetric flow rate of the liquid agent (mL/min)
ρ = density of the liquid agent (g/mL)
$MW_{liq\ agent}$ = molecular weight of the liquid agent (g/mole)

The molar flow rate of air is determined using Equation (4). The extinguishment concentration in volume percent is calculated according to Equation (2). When calculating liquid agent extinguishment concentrations, pressure and temperature are important since the values for $n_{liq\ agent}$ and n_{air} are used in the calculation.

Cup-burner results are usually given as the minimum gas-phase concentration needed to suppress a flame. One can then relate the result to a reference compound to calculate a Gas Volume Equivalent (GVEq). For example, if a candidate agent has an extinguishment concentration of EC_C and a reference compound has an extinguishment concentration of EC_R, then the GVEq is given by Equation (7):

$$GVEq = EC_C/EC_R \tag{7}$$

Note that the GVEq gives the increase in gaseous volume of a candidate agent as needed to provide an extinguishment as measured by a cup burner equivalent to the reference agent. The reciprocal of the GVEq gives the Gas Volume Effectiveness (GVEf), which is the effectiveness of a candidate material relative to the reference compound (Equation 8). For GVEq, a higher number indicates a lower efficiency. The opposite is true for GVEf.

$$GVEf = 1/GVEq = EC_R/EC_C \tag{8}$$

The gas-phase concentration of an agent required to extinguish a flame does not always provide an accurate representation of an agent's efficiency. More important are the weight and storage volume of an agent required to give the same fire extinguishment capability as a

reference compound. The Weight Equivalent (WEq) is the ratio of the weight of the candidate agent to the weight of the reference agent. The equation used is

$$WEq = GVEq \times (MW_C/MW_R) = (EC_C/EC_R) \times (MW_C/MW_R) \quad (9)$$

where "MW" denotes "molecular weight," the subscript "C" denotes "candidate," and the subscript "R" denotes "reference agent." The Weight Effectiveness (WEf) is the reciprocal of the WEq and gives a measure of the effectiveness of a candidate relative to that of the reference material as determined by the weight required to suppress a cup-burner flame (Equation 10).

$$WEf = 1/WEq = 1/GVEq \times (MW_R/MW_C) = (EC_R/EC_C) \times (MW_R/MW_C) \quad (10)$$

Note that as the molecular weight of the candidate agent increases, the WEq increases and the WEf decreases. Thus, lower molecular weight materials appear to be more effective when effectiveness is measured by weight. Like the numbers for gas volume, a higher efficiency is denoted by a higher WEf and a lower WEq.

The Storage Volume Equivalent (SVEq) is the amount of candidate agent as measured by storage volume requirements relative to that required by a reference agent. The storage density of the agent is important in determining the storage volume requirements. Obviously, a higher density means that less space is required. Since most agents of interest here are stored as liquids (usually under pressure) because they require less volume, liquid densities (LD) are used to determine the SVEq (Equation 11).

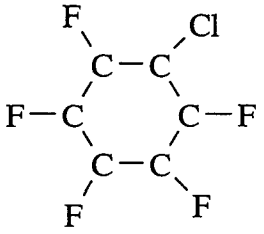
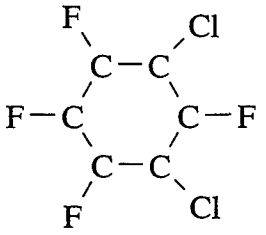
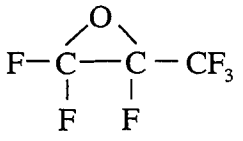
$$SVEq = WEq \times (LD_R/LD_C) = (EC_C/EC_R) \times (MW_C/MW_R) \times (LD_R/LD_C) \quad (11)$$

Again, one can use the Storage Volume Effectiveness (SVEf) to measure the effectiveness relative to a reference compound (Equation 12).

$$SVEf = 1/SVEq = (EC_R/EC_C) \times (MW_R/MW_C) \times (LD_C/LD_R) \quad (12)$$

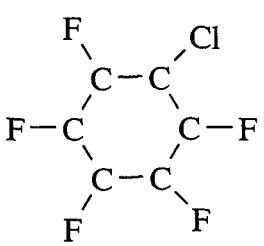
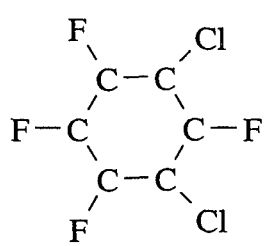
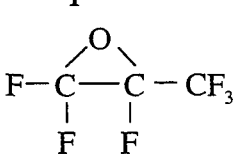
All of the cup-burner work reported herein employed *n*-heptane as the fuel. Average extinguishment concentrations for the materials tested are presented in Table 10. Many of these chemicals were tested to gain an understanding of the fire suppression mechanism and to develop a database for predictive algorithm generation—not addressed in this project. Table 11 presents the GVEq, WEq, and SVEq of each of the chemicals considered as Halon 1211 replacements. As indicated above, lower GVEq, WEq, and SVEq values denote more effective chemicals, in comparison to Halon 1211. Values of unity suggest that the chemical is equally as effective as halon. Caution should be taken, however, when selecting streaming agents based on cup-burner values alone (Reference 19).

TABLE 10. CUP-BURNER TEST RESULTS.

Compound	Test Method	[a]Ext. Conc. Volume %
CF_3I	Gas	3.0
CF_3CF_2I	Gas	2.1
$CF_3CF_2CF_2I$	Liquid	3.0
CF_3CFICF_3	Liquid	3.2
$CF_3CF_2CF_2CF_2I$	Liquid	2.8
$CF_3CF_2CF_2CF_2CF_2CF_2I$	Liquid	2.5
$CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_2I$	Liquid	1.9
$CF_2ICF_2CF_2CF_2I$	Liquid	2.1
$CHBr=CHCF_3$	Liquid	[b]8.5
$CH_2=CBrCF_3$	Liquid	2.6
$CH_2=CHCBrF_2$	Liquid	4.5
$CH_2=CHCClFCBrF_2$	Liquid	4.5
$CH_2=CHCF_2BrCF_2$	Liquid	3.5
	Liquid	5.4
	Liquid	6.0
	Gas	9.6

[a] NMERI 5/8-scale cup-burner apparatus with n-heptane as the fuel.
[b] Insufficient quantity for accurate testing.

TABLE 11. CANDIDATE FIRE SUPPRESSION EFFECTIVENESS.

Compound	MW (amu)	Liq. Dens (g/mL)	[a]Ex. Con. (vol %)	GVEq	WEq	SVEq
CF_3I	195.91	2.10	3.0	0.93	1.10	0.96
CF_3CF_2I	245.92	2.09	2.1	0.65	0.97	0.85
$CF_3CF_2CF_2I$	295.92	2.06	3.0	0.93	1.67	1.48
CF_3CFICF_3	295.93	2.08	3.2	0.99	1.78	1.56
$CF_3CF_2CF_2CF_2I$	345.93	2.01	2.8	0.87	1.82	1.66
$CF_3CF_2CF_2CF_2CF_2CF_2I$	445.95	2.05	2.5	0.78	2.09	1.87
$CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_2I$	545.97	---	1.9	0.59	1.95	---
$CF_2ICF_2CF_2CF_2I$	453.84	2.50	2.1	0.66	1.80	1.32
$CHBr{=}CHCF_3$	174.95	---	[b]8.5	[b]2.64	[b]2.79	---
$CH_2{=}CBrCF_3$	174.95	1.69	2.6	0.81	0.85	0.92
$CH_2{=}CHCBrF_2$	156.96	1.54	4.5	1.40	1.33	1.57
$CH_2{=}CHCClFCBrF_2$	223.40	1.68	4.5	1.40	1.89	2.06
$CH_2{=}CHCF_2CBrF_2$	206.96	1.36	3.5	1.09	1.36	1.83
	202.51	1.57	5.4	1.68	2.05	2.40
	218.97	1.65	6.0	1.86	2.47	2.73
	166.02	NA	9.6	2.98	2.99	NA

[a] NMERI 5/8-scale cup-burner apparatus with *n*-heptane as the fuel.
[b] Insufficient quantity for accurate testing.

SECTION V
CONCLUSIONS AND RECOMMENDATIONS

Of the agents reported within this scope of work, heptadecafluoro-1-iodooctane ($CF_3CF_2CF_2CF_2CF_2CF_2CF_2CF_2I$), pentafluoroiodoethane (CF_3CF_2I), and octafluoro-1,4-diiodobutane ($CF_2ICF_2CF_2CF_2I$) have the lowest extinguishment concentrations by volume percent. The agents with the best weight equivalents (WEq) and storage volume equivalents (SVEq) in relation to Halon 1211 are 2-bromo-3,3,3-trifluoro-1-propene ($CH_2=CBrCF_3$), pentafluoroiodoethane (CF_3CF_2I), and trifluoroiodomethane (CF_3I). All three agents have better SVEqs, and two of the agents (pentafluoroiodoethane and 2-bromo-3,3,3-trifluoro-1-propene) have better WEqs. The remaining agents had significantly higher SVEqs (32 percent greater or more) and WEqs (33 percent greater or more).

Although no tropodegradable replacement with a toxicity as low as that of Halon 1301 or 1211 has yet been identified, the results look very promising. A number of these agents are expected to have zero or near zero ozone-depletion potentials (ODP). For example, one agent, trifluoromethyliodide (CF_3I), is as effective as Halon 1301 and has an atmospheric lifetime of less than one day (Reference 5).

One group of tropodegradable chemicals not studied in this initial investigation are the polar-substituted compounds. These include compounds with carbonyl groups (ketones, aldehydes, esters, carboxylic acids), compounds with hydroxyl groups (alcohols), ethers (particularly HFE derivatives), and amines, amides, and morpholines. Studies of these compounds is strongly recommended.

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REFERENCES

1. "Number Designation and Safety Classification of Refrigerants," ANSI/ASHRAE Standard 34-1992, American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, Georgia, 1992.

2. Dekleva, T., "Recommended Convention for Naming Ether Refrigerants," Nomenclature Subcommittee, ASHRAE SSPC 34, 20 October 1994.

3. Skaggs, S. R., and Tapscott, R. E., *Advanced Streaming Agent Program: Candidate Survey*, Final Report, Wright Laboratories, Tyndall Air Force Base, Florida and Applied Research Associates, Inc., Tyndall Air Force Base, Florida, December 1994. NMERI 1994/45 (Draft)

4. Huie, R. E., and Laszlo, B., "The Atmospheric Chemistry of Iodine Compounds," in *Halon Replacements, Technology and Science*, ACS Symposium Series 611, Miziolek, A. W. and Tsang, W., editors, American Chemical Society, Washington, DC, 4, pp. 31-40, 1995.

5. Moore, T. A., Skaggs, S. R., Corbitt, M. R., Tapscott, R. E., Dierdorf, D. S., and Kibert, C. J., *The Development of CF_3I as a Halon Replacement*, Wright Laboratories, Tyndall Air Force Base, Florida, November 1994. NMERI 1994/40 (Draft)

6. Nimitz, J. S., and Lankford, L., "Fluoroiodocarbons as Halon Replacements," *Proceedings, International CFC and Halon Alternatives Conference*, Washington, DC, pp. 810-819, 20-22 October 1993.

7. Kibert, C. J., "Fluoroiodocarbons as Halon 1211/1301 Replacements: An Overview," *Proceedings, Halon Options Technical Working Conference*, pp. 261-269, 3-5 May 1994, Albuquerque, New Mexico.

8. McIlroy, A., "Ignition Suppression by CF3Br and CF3I of H2/O2/Ar Mixtures: Detailed Studies of Time and Space Resolved Radical Profiles," *Proceedings, Halon Options Technical Working Conference*, pp. 271-282, 3-5 May 1994, Albuquerque, New Mexico.

9. Nimitz, J. S., "Trifluoromethyl Iodide and its Blends as High-Performance, Environmentally Sound Halon 1301 Replacements," *Proceedings, Halon Options Technical Working Conference*, pp. 283-294, Albuquerque, New Mexico, 3-5 May 1994.

10. Tapscott, R. E., Moore, T. A., Skaggs, S. R., and Heinonen, E. W., *Fluoroiodide Blends as Streaming Agents: Selection Criteria and Cup-Burner Results*, Wright Laboratories and Applied Research Associates, Inc., Tyndall Air Force Base, Florida, June 1995. NMERI 1995/8/31790

11. Oomure, U., Noguchi, M., Ide, S., and Momota, H., "Halo Hydrocarbon-Containing Fire Extinguishers," Japanese Patent 05 42230 [93 42,230], February 23, 1993 (*Chemical Abstracts*, Vol. 119, No. 52487j).

12. Merchant, A. N., and Sung, J. C., "Binary Azerotropic Compositions of 1,1,2,2,3,3,4,4-Octafluorobutane and Either Trans-1,2-dichloroethylene, Cis-1,2-dichloroethylene, or 1,1-Dichloroethane," U.S. Patent 5,194,170, March 16, 1993 (*Chemical Abstracts*, Vol. 119, No. 30430h).

13. Merchant, A. N., "Binary Azeotropic Compositions of 1,1-Dichloro-1-fluoroethane and (*n*-Perfluorobutyl)ethylene," U.S. Patent 5,037,573, August 6, 1991 (*Chemical Abstracts*, Vol. 115, No. 235186x).

14. Shekhtmeister, I. E., Ivanov, V. M., Beilina, V. I., Kusheverskaya, S. V., "Preparation of Self-Extinguishing Polystyrene Foam by the Surface Treatment of Unfoamed Beads," Plast. Massy, pp. 57-58, 1981 (*Chemical Abstracts*, Vol. 95, No. 20483w).

15. Di Bella, E. P., Keyworth, D. A., Rosen, M., "Flame-Retardant Emulsion Containing 1,1,2,3,4,4-hexabromobut-2-ene," U.S. Patent 3,981,806, September 21, 1976 (*Chemical Abstracts*, Vol. 86, No. 18314r).

16. Nimitz, J. S., Tapscott, R. E., and Skaggs, S. R., "Next-Generation High-Efficiency Halon Replacements," International CFC and Halon Alternatives Conference, Baltimore, Maryland, 10 pages, December 3-5, 1991.

17. Robin, M. L., "Halogenated Fire Suppression Agents," in *Halon Replacements, Technology and Science*, ACS Symposium Series 611, Miziolek, A. W. and Tsang, W., editors, American Chemical Society, Washington, DC, 9, pp. 85-98, 1995.

18. Tapscott, R. E., May, J. H., Moore, J. P., Lee, M. E., and Walker, J. L., *Next Generation Fire Extinguishing Agents Phase II – Laboratory Tests and Scoping Trials*, ESL-TR-87-03, Vol. 2 of 5, Air Force Engineering and Services Laboratory, Tyndall AFB, Florida, April 1990.

19. Moore, J. P., Moore, T. A., Salgado, D. P., and Tapscott, R. E., "Halon Alternatives Extinguishment Testing," International Conference on CFC and Halon Alternatives, Washington, DC, 8 pages (unpublished), October 10-11, 1989.

APPENDIX A
MATERIAL PROPERTY SHEETS

The following sheets are presented in the order established in Table 1 (under IUPAC Name). Material property sheets are not provided for the following:

4-Bromo-3-chloro-3,4,4-trifluoro-1-butene

4-Bromo-3,3,4,4-tetrafluoro-1-butene

Chloropentafluorobenzene

1,3-Dichloro-2,4,5,6-tetrafluorobenzene

Trifluoro(trifluoromethyl)oxirane

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 100

IUPAC Name:	trifluoroiodomethane
Formula:	CF3I
Common/Trade Name(s):	Triodide (Pacific Scientific); Iodoguard (West Florida Ordnance)
CAS Number:	2314-97-8
Empirical Formula:	CF3I
Molecular Weight:	195.911
Halon Number:	13001
Halocarbon No.:	FIC-13I1
Blend Composition:	Pure Compound
Comments:	Vapor pressure curve: log P (psia) = 5.7411 - 1146.82/T(K)

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):	0.005	<0.005	437
ODP (relative to CFC-11):	0.0001	Maximum: <0.008; Likely: <0.0001	6065
GWP:	1	<<1: 100-yr CO2(<5: 20-yr; <<<1: 500-yr	437
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):	62	25°C	6688
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:	7.066178	Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 100

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):	12.8	ALC > 12.8%	6688
AEL (ppm):			
NOAEL (%):	0.2	beagle, cardiac sensitization	6054
LOAEL (%):	0.4	beagle, cardiac sensitization	6054
TSCA Listed?:			
Toxicology Notes:	During acute LC50 studies, rats exhibited anesthesia, salivation, and audible respiration.		

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	-22.5	1 atm	2119
Melting Point (°C):	-110	estimated value from NIST, 1995	
Critical Pressure (bar):	40.41	4041 kPa	6688
Critical Temperature (°C):	122	estimated	6056
Critical Density (g/mL):	0.8706	225 mL/mol	6688
Vapor Density at 25°C (g/L):	8.013	Calculated	
Liquid Density (g/mL):	2.096	20 to 25°C	6056
Refractive Index:	1.379	-42°C	2119
AzTemp:			
Vapor Pressure (bar):	4.392	25°C	6688
Liquid Viscosity (cp):	0.198	25°C	6688
Vapor Viscosity (cp):			
Dipole Moment (Debye):	1.68	AMPAC Calculation	
Ionization Potential (eV):	11.97	AMPAC Calculation	
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 100

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):	-2990.64		787
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):	112.4	@ boiling point	6688
Liquid Heat Capacity (J/kg):	592	25°C	6688
Vapor Heat Capacity (J/kg):	361.8	25°C, 1 atm	2110
Liq. Thermal Conductivity (W/m K):	0.07	25°C	6688
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	3.02	full confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):	1.36		6189
Storage Volume Equivalent (SVEq):	0.87		6189
Inertion Conc., Methane (% by vol):	3.1		6188
Inertion Conc., Propane (% by vol):	5.2	6.5% flammability peak, ref 6054	6188
Flash Point (°C):		none	6056
LFL or LEL (% by vol):		nonflammable	6056
UFL or UEL (% by vol):		nonflammable	6056
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 881

IUPAC Name: pentafluoroiodoethane

Formula: CF3CF2I

Common/Trade Name(s): perfluoroethyl iodide

CAS Number: 354-64-3

Empirical Formula: C2F5I

Molecular Weight: 245.91

Halon Number: 25001

Halocarbon No.: FIC-115I1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 881

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:	Yes		
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	12		6189
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	10.058	Calculated	
Liquid Density (g/mL):	2.085		6189
Refractive Index:	1.3378	0.5 °C	3298
AzTemp:			
Vapor Pressure (bar):	0.956	9.8°C	2618
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):	1.6	AMPAC Calculation	
Ionization Potential (eV):	11.962	AMPAC Calculation	
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 881

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):	-914.16	AMPAC Calculation	
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):	448.5		2110
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	2.09	full confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):	0.98	relative to Halon 1211	6189
Storage Volume Equivalent (SVEq):	0.96	relative to Halon 1211	6189
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):	11		6188
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 882

IUPAC Name: heptafluoro-1-iodopropane

Formula: CF3CF2CF2I

Common/Trade Name(s): perfluoro-n-propyl iodide, heptafluoropropyl iodide, heptafluoro-1-iodopropane

CAS Number: 754-34-7

Empirical Formula: C3F7I

Molecular Weight: 295.92

Halon Number: 37001

Halocarbon No.: FIC-217cal1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:	6.517989	Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 882

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:			
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	41.2		2619
Melting Point (°C):	-95.3		2619
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	12.103	Calculated	
Liquid Density (g/mL):	2.0626		2619
Refractive Index:	1.3281		2619
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):	1.77	AMPAC Calculation	
Ionization Potential (eV):	11.959	AMPAC Calculation	
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 882

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):	-1063.64	AMPAC Calculation	
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):	94.62		2794
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):	665.7		2794
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	3.04	full confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):	1.68	relative to Halon 1211	6189
Storage Volume Equivalent (SVEq):	1.66	relative to Halon 1211	6189
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):	7.6	7.6±0.4, small sample size	6188
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 430

IUPAC Name: 1,1,1,2,3,3,3-heptafluoro-2-iodopropane

Formula: CF3CFICF3

Common/Trade Name(s): heptafluoropropyl iodide; perfluoroisopropyl iodide;

CAS Number: 677-69-0

Empirical Formula: C3C7I

Molecular Weight: 295.926

Halon Number: 37001

Halocarbon No.: FIC-217baI1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 430

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:	Yes		6518
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	38	38 to 40°C	6189
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	12.103	Calculated	
Liquid Density (g/mL):	2.08		6518
Refractive Index:	1.3295	20°C	6518
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):	1.83	AMPAC Calculation	
Ionization Potential (eV):	12.064	AMPAC Calculation	
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 430

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):	-1086.76	AMPAC Calculation	
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	3.15	full confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):	1.79	relative to Halon 1211	6189
Storage Volume Equivalent (SVEq):	1.74	relative to Halon 1211	6189
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):		none	6518
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 276

IUPAC Name: nonafluoro-4-iodobutane

Formula: CF3CF2CF2CF2I

Common/Trade Name(s): perfluorobutyl iodide

CAS Number: 423-39-2

Empirical Formula: C4F9I

Molecular Weight: 345.93

Halon Number: 49001

Halocarbon No.: FIC-319I1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 276

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:	Yes		
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	67	also 68	6189
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	14.148	Calculated	
Liquid Density (g/mL):	2.01		6189
Refractive Index:	1.3285	@ 20°C	6518
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 276

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	2.8	full confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):	4.9	4.9±0.6	6188
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 180

IUPAC Name: 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-1-iodohexane

Formula: CF3CF2CF2CF2CF2CF2I

Common/Trade Name(s): tridecafluorhexyl iodide

CAS Number: 355-43-1

Empirical Formula: C6F13I

Molecular Weight: 445.95

Halon Number: 6-13-0-0-1

Halocarbon No.: FIC-5-1-13I1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 180

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:	Yes		
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	117		6189
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	18.239	Calculated	
Liquid Density (g/mL):	2.05		6189
Refractive Index:	1.3275	@ 20°C	6518
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 180

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	2.5	full confidence	6189
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):	2.11		6189
Storage Volume Equivalent (SVEq):	2.1		6189
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 344

IUPAC Name:	1,1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8-heptadecafluoro-8-iodooctane
Formula:	CF2ICF2CF2CF2CF2CF2CF2CF3
Common/Trade Name(s):	perfluorooctyl iodide; heptadecafluoro-1-iodooctane
CAS Number:	507-63-1
Empirical Formula:	C8F17I
Molecular Weight:	545.97
Halon Number:	8-17-0-0-1
Halocarbon No.:	FIC-7-1-17II1
Blend Composition:	Pure Compound
Comments:	For 6519 references, this compound can be found using this identification code H-90006.

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 344

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:	Yes		6518
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	160	161°C Also measured at 95°C @ 103 m	6519
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	22.33	Calculated	
Liquid Density (g/mL):			
Refractive Index:	1.3306	20°C	6518
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 344

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):			
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 874

IUPAC Name: 1,1,2,2,3,3,4,4-octafluoro-1,4-diiodobutane

Formula: CF2ICF2CF2CF2I

Common/Trade Name(s): octafluoro-1,4-diiodobutane

CAS Number: 375-50-8

Empirical Formula: C4F8I2

Molecular Weight: 453.84

Halon Number: 48002

Halocarbon No.: FIC-318IccI2

Blend Composition: Pure Compound

Comments: Info obtained from MSDS, Japan Halon Co.

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 874

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:			
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	85		
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	18.562	Calculated	
Liquid Density (g/mL):	2.5		
Refractive Index:			
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 874

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	3		374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 707

IUPAC Name: 1-bromo-3,3,3-trifluoropropene

Formula: CHBr=CHCF3

Common/Trade Name(s):

CAS Number:

Empirical Formula: C3H2BrF3

Molecular Weight: 174.95

Halon Number:

Halocarbon No.: HBFC-1233zdB1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 707

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:			
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	40		3915
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	7.155	Calculated	
Liquid Density (g/mL):			
Refractive Index:			
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 707

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	8.5	Limited Confidence	374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 873

IUPAC Name: 2-bromo-3,3,3-trifluoropropene

Formula: CH2=CBrCF3

Common/Trade Name(s):

CAS Number: 1514-82-5

Empirical Formula: C3H2BrF3

Molecular Weight: 174.95

Halon Number:

Halocarbon No.: HBFC-1233xfB1

Blend Composition: Pure Compound

Comments: Info obtained from MSDS, Japan Halon Co.

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 873

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:			
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	34	34 to 35°C	
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	7.155	Calculated	
Liquid Density (g/mL):	1.69	@16°C	
Refractive Index:			
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 873

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):	2.55		374
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 872

IUPAC Name: 3-bromo-3,3-difluoropropene

Formula: CH2=CHCBrF2

Common/Trade Name(s):

CAS Number: 420-90-6

Empirical Formula: C3H3BrF2

Molecular Weight: 156.96

Halon Number:

Halocarbon No.: HBFC-1242zfB1

Blend Composition: Pure Compound

Comments:

Environmental Data

Parameter	Value	Condition	Ref.
Atmospheric Lifetime (yrs):			
ODP (relative to CFC-11):			
GWP:			
Temperature Sensitivity:			

Solubility Data

Parameter	Value	Condition	Ref.
Solubility in Water (ppm):			
Solubility of Water (ppm):			
Henry's Constant (L atm/mol):			
Log Octanol-Water Partition:			
Hildebrand Parameter (cal/cm3)½:		Calculated Hildebrand Parameter at 25°C.	

CHEMICAL OPTIONS DATABASE: CHEMICAL ID = 872

Inhalation Toxicity Data and Exposure limits

Parameter	Value	Condition	Ref.
OSHA PEL or EPA WGL (ppm):			
AICGH TLV or AIHA WEEL (ppm):			
OSHA STEL or Ceiling (ppm):			
NIOSH IDLH or EPA EGL (ppm):			
LC50 or ALC (%):			
AEL (ppm):			
NOAEL (%):			
LOAEL (%):			
TSCA Listed?:			
Toxicology Notes:			

Physical Properties:

Parameter	Value	Condition	Ref.
Boiling Point (°C):	4		
Melting Point (°C):			
Critical Pressure (bar):			
Critical Temperature (°C):			
Critical Density (g/mL):			
Vapor Density at 25°C (g/L):	6.42	Calculated	
Liquid Density (g/mL):			
Refractive Index:			
AzTemp:			
Vapor Pressure (bar):			
Liquid Viscosity (cp):			
Vapor Viscosity (cp):			
Dipole Moment (Debye):			
Ionization Potential (eV):			
Liquid Dielectric Constant:			
Vapor Dielectric Constant:			
Thermal Expansion Coefficient:			

CHEMICAL OPTIONS DATABASE:
CHEMICAL ID = 872

Thermodynamic Data

Parameter	Value	Condition	Ref.
Heat of Formation (kJ/kg):			
Heat of Combustion (kJ/kg):			
Heat of Vaporization (kJ/kg):			
Liquid Heat Capacity (J/kg):			
Vapor Heat Capacity (J/kg):			
Liq. Thermal Conductivity (W/m K):			
Vap. Thermal Conductivity (W/m K):			

Extinguishment and Flammability Data

Parameter	Value	Condition	Ref.
5/8 Cup Burner, n-heptane (%):			
Other Cup Burner, n-heptane (%):			
Gas Volume Equivalent (GVEq):			
Weight Equivalent (WEq):			
Storage Volume Equivalent (SVEq):			
Inertion Conc., Methane (% by vol):			
Inertion Conc., Propane (% by vol):			
Flash Point (°C):			
LFL or LEL (% by vol):			
UFL or UEL (% by vol):			
Autoignition Temperature (°C):			