

IDENTIFICATION OF CFC AND HCFC SUBSTITUTES FOR
BLOWING POLYURETHANE FOAM INSULATION PRODUCTS

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16. ABSTRACT The report gives results of a cooperative effort to identify chlorofluorocarbon (CFC) and hydrochlorofluorocarbon (HCFC) substitutes for blowing polyurethane foam insulation products. The substantial ongoing effort is identifying third-generation blowing agents for polyurethane foams to replace currently used stratospheric ozone depleting ones. More than 100 chemicals have been identified and ranked as polyurethane foam blowing agent candidates. The systematic investigation involved the analysis of vapor thermal conductivity predictive models and utilizing this methodology to identify and screen potential new foam blowing agents. Collection of physical/chemical properties of the new candidates enabled an overall evaluation. Based on the vapor thermal conductivity, boiling point, and other important properties, the chemical compounds were ranked to identify the most promising new blowing agent candidates. To efficiently evaluate new foam blowing agents, the compounds were placed and evaluated in 14 groups based on chemical structure. Compounds ranked high in this exercise included cyclopentane and cyclopentene, simple olefins consisting of hydrocarbons with four to six carbons and at least one double bond, cyclobutane analogs, and fluorinated propanes and butanes. Several novel chemical groups, such as fluoroiodoalkanes and silicon compounds, were also considered and ranked.		
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FOREWORD

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National Risk Management Research Laboratory

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Abstract

Substantial effort is ongoing to identify and evaluate third-generation blowing agents for polyurethane foams to replace currently used stratospheric ozone depleting ones. A cooperative agreement between the Environmental Protection Agency and Syracuse Research Corporation has identified and ranked over 100 chemicals as polyurethane foam blowing agent candidates. The systematic investigation involved the analysis of vapor thermal conductivity predictive models and utilizing this methodology to identify and screen potential new foam blowing agents. Collection of physical/chemical properties of the new candidates enabled an overall evaluation. Based on the vapor thermal conductivity, boiling point, and other important properties, the chemical compounds were ranked in order to identify the most promising new blowing agent candidates. In order to efficiently evaluate new foam blowing agents, the compounds were placed and evaluated in a series of fourteen groups based on chemical structure. Compounds ranked high in this exercise included cyclopentane and cyclopentene, simple olefins consisting of hydrocarbons with 4 to 6 carbons and at least one double bond, cyclobutane analogs, and fluorinated propanes and butanes. Several novel chemical groups, such as fluoroiodoalkanes and silicon compounds, were also considered and ranked in the exercise.

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Introduction

Chlorofluorocarbons (CFCs) are recognized as a major contributor to the depletion of stratospheric ozone in the Earth's atmosphere. Stratospheric ozone helps to filter harmful ultraviolet (UV) radiation and decreases the amount that reaches the Earth's surface. Because of the potential for harm to health or the environment as a result of the increased incidence of UV radiation, the phaseout of production of this class of chemicals was called for as of January 1, 1996, under the auspices of the Montreal Protocol and current U.S. law. CFCs were widely used as blowing agents for rigid polyurethane foams for insulation products due to their unique combination of desirable physical/chemical properties and safety in use.

Worldwide efforts to replace CFC blowing agents led to the development of the so-called second-generation blowing agents, the hydrochlorofluorocarbons, HCFCs (Knopeck, GM. et al., 1993; Decaire, BR. et al., 1992). HCFCs have significantly lower ozone depletion potentials compared to CFCs and many of these second-generation blowing agents could be used directly as drop-in replacements for CFCs. HCFCs, however, also face phase-out under the Montreal protocols and subsequent agreements due to their contribution to stratospheric ozone depletion and thus, they represent only an interim replacement for CFCs.

There is a need to identify chemical compounds that are not stratospheric ozone depleters that can be used as substitutes for CFC and HCFC blowing agents in rigid polyurethane foam insulating materials. The search for these compounds is complicated by the physical/chemical properties they must possess as well as their overall compatibility with foam feedstocks and production methods. Subtle differences between the third-generation blowing agents and CFCs or HCFCs may result in modification in production methods as well as differences in use and utility of the foam product.

Substantial effort has been expended by governmental, industrial, and private laboratories to test and evaluate a small number of third-generation blowing agents. This project was designed to identify additional polyurethane foam blowing agent candidates in order to improve the chances of finding successful ones by conducting a systematic search to identify new compounds that could replace the CFCs and HCFCs currently in use.

This final report represents the findings under Tasks 1, 2, and 3 of the project entitled Identification of CFC and HCFC Substitutes for Blowing Polyurethane Foam Insulation Products. Task 1 involved the analysis of vapor thermal conductivity predictive models. The vapor thermal conductivity of the blowing agent is an important physical property for insulating materials because the blowing agent becomes incorporated into the foam and, therefore, is partially responsible for hindering the movement of heat through the foam. Given that experimental vapor thermal conductivity values are essentially limited to currently available blowing agents and refrigerants (which are mostly CFCs and HCFCs) and that experimental measurements on a large number of compounds would be economically prohibitive, a model to rapidly screen a large number of compounds would be advantageous in identifying new blowing agents. This task involved the evaluation of current models for estimating vapor thermal conductivity, fine tuning the models to reflect the current body of knowledge in this area, and utilizing this methodology to identify and screen potential new foam blowing agents.

Task 2 involved the identification of potential new foam blowing chemicals and their properties and the collection of physical/chemical properties and other data on the new candidates. Based on the vapor thermal conductivity, boiling point, and other important properties of each candidate, the chemical compounds identified in this task were ranked in order to identify the most promising new blowing agent candidates. Task 3 involved the evaluation of

potential new foam blowing agents as groups of related candidates. By placing candidates in chemical groups, similarities could be discussed collectively and trends that represent differences could be identified.

Task 1: Analysis of Vapor Thermal Conductivity Predictive Models

The vapor thermal conductivity of a blowing agent for an insulating foam is an important factor in its overall insulating ability. Because of this, the vapor thermal conductivity is an important chemical property to consider when looking at potential blowing agent substitutes. Experimental data on vapor thermal conductivities are lacking in the open literature, except for established blowing agents and refrigerants. Therefore, a significant portion of this project was to establish the reliability of vapor thermal conductivity predictive models.

Two attributes of a gas enter into its thermal conductivity; how much heat the gas can absorb, and how fast the gas can transport the heat from one surface to another (its diffusivity). Absorption is dependent upon the heat capacity of the gas. Since heat is stored in bond vibrations, the greater the number of bonds, the greater the heat capacity, all else being equal.

Thermal conductivity decreases with increasing critical temperature, which is the highest temperature at which the gas can exist as a liquid. This dependence is complex since critical temperature is related to both the absorption of heat by the gas and its translational motion. In contrast, thermal conductivity increases with increasing critical pressure, which is directly related to diffusivity.

The best potential blowing agent, in terms of low thermal conductivity, is one which provides the best compromise between high critical temperature and low critical pressure, and is

relatively bulky, yet has a low enough boiling point. Heat capacity is most favorable for halogens, carbonyls, and ethers, and not for saturated hydrocarbons, alcohols, or amines.

The calculation of thermal conductivity, λ , requires a knowledge of the Roy-Thodos constant C, which is estimated from group contribution values. Unfortunately, rules for calculating these contributions are not well developed as shown from the following examples.

Thermal Conductivity

Thermal conductivity was estimated by the Roy-Thodos method (Roy, D. and Thodos, G., 1968; Roy, D. and Thodos, G., 1970). Four input parameters are required:

- T_c - the critical temperature, in K;
- P_c - the critical pressure, in bars;
- C - a compound-specific constant estimated by a group contribution scheme; and
- M - the molecular weight in g/mol.

T_r is the reduced temperature, i.e., T/T_c , both in K.

The thermal conductivity (λ) is expressed as

$$\lambda = \lambda_r / \Gamma$$

where λ_r is the reduced thermal conductivity, and Γ represents the reduced inverse thermal conductivity in units of $[\text{mW}/(\text{m K})]^{-1}$. Γ is calculated from

$$\Gamma = 210 (T_c M^3 / P_c^4)^{1/6}$$

The reduced thermal conductivity, λ_r , has a translational and an internal component, i.e.,

$$\lambda_r = (\lambda\Gamma)_{tr} + (\lambda\Gamma)_{int}$$

The translational component is computed according to

$$(\lambda\Gamma)_{tr} = 8.757 [\exp(0.0464T_r) - \exp(-0.2412T_r)]$$

The internal part of the reduced thermal conductivity is calculated through

$$(\lambda\Gamma)_{int} = C f(T_r)$$

where $f(T_r)$ is chemical class specific, and is given by various equations containing terms in T_r .

For example, for halides, the following equation applies

$$f(T_r) = -0.107 T_r + 1.330 T_r^2 - 0.223 T_r^3$$

Other equations are available for saturated hydrocarbons; olefins; acetylenes; naphthalenes and aromatics; alcohols, aldehydes, ethers, and esters; amines and nitriles; and cyclic compounds.

The term “C” is a group contribution parameter that is obtained from the nature and number of functional groups and their regiochemistry.

There are two difficulties with the technique. One is that since $f(T_r)$ is chemical class specific, there is no obvious solution if the structure falls into more than one chemical class. For example, several of the structures considered were haloethers, and technically, either the equation for halides or ethers could be used. We used the equation for halides, since the structures usually contained several halo groups but usually only a single ether linkage. In a few cases, calculations were made with both equations and the results were similar.

The other difficulty lies with the estimation of C. For example, one equation governs cyclic compounds, whereas another deals with halides, but there is no explicit equation for cyclic halogenated compounds. Also, an equation exists for bromine substitution on methane, but not for bromine substitution on anything else. In these cases, a near-neighbor approach was used if the missing fragment was closely related to a listed species; otherwise, the structure could not be considered further as a potential blowing agent substitute for this project.

In order to evaluate the reliability of the Roy-Thodos method for estimating thermal conductivity, estimated values were directly compared to available experimental values. Figure 1 provides a comparison between experimental vapor thermal conductivity values obtained from Daubert and Danner's compilation (Daubert, TE., and Danner, RP., 1989) to our estimated


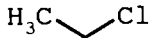
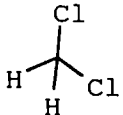
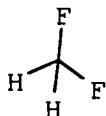
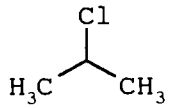
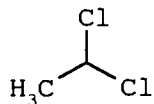


Figure 1. Estimated vs. Experimental Vapor Thermal Conductivity

values. As can be seen in Figure 1, the estimated vapor thermal conductivities were generally within 10% of the experimental values for the chemicals listed in Daubert and Danner that had experimental values. In addition, the estimated values were typically lower than the experimental ones (bars above the line in Figure 1). Figure 1 also demonstrates that no generalization can be developed regarding the potential magnitude and direction for the differences between experimental and estimated values based on structure, functionality, or substitution patterns. From these results, the overall accuracy of the Roy-Thodos model for predicting vapor thermal conductivity was good enough to use these estimated values where used directly in the second phase of this project.

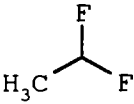
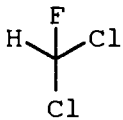
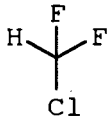
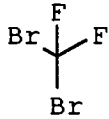
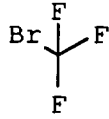
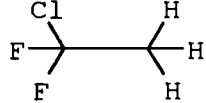
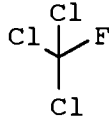
Table 1 contains a complete list of experimental and estimated vapor thermal conductivity values in $\text{mW}/(\text{m K})$ collected during this phase of the project and are sorted by CAS Registry numbers. There are 51 experimental vapor thermal conductivity values at or near room temperature ($25\text{ }^{\circ}\text{C}$) in Table 1 that were collected from the open literature during this phase of the task. A statistical analysis of the experimental and estimated vapor thermal conductivities for these 51 compounds reveals a correlation coefficient (r^2) of 0.82, a standard deviation of $.00952 \times 10^{-1} \text{ mW}/(\text{m K})$, and an absolute mean error of $.00691 \times 10^{-1} \text{ mW}/(\text{m K})$. Figure 2 provides a graphical representation of these results. In Figure 2, there are clearly two outliers in this data set corresponding to 1,1,1-trichloro-2,2,2-trifluoroethane and 1-chloro-1,1,2,2,2-pentafluoroethane. When these outliers are removed from the statistical analysis, a correlation coefficient of 0.89, a standard deviation of $.00719 \times 10^{-1} \text{ mW}/(\text{m K})$, and an absolute mean error of $.00588 \times 10^{-1} \text{ mW}/(\text{m K})$ is obtained. Further analysis of Figure 2 shows that the estimated results for compounds with thermal conductivities ranging from 8 to 13

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000067641	Acetone	12.00	0.00	0.00		
000074873	Methane, chloro-	11.30	10.70	10.50 20	Suh, KW. (1994)	$\text{H}_3\text{C}-\text{Cl}$
000075003	Ethane, chloro-	11.90	11.40	8.87 0	Missenard, FA. (1966)	
∞ 000075092	Methane, dichloro-	8.01	7.41	6.30 20	Suh, KW. (1994)	
000075105	Methane, difluoro-	11.10	11.00	12.80 25	Suehla, RA. (1962)	
000075296	Propane, 2-chloro-	11.70	11.50	0.00		
000075343	Ethane, 1,1-dichloro-	9.68	9.40	0.00		

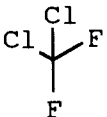
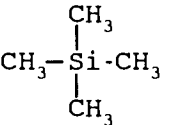
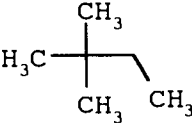
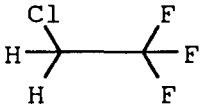
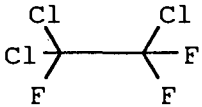
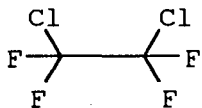
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000075376	Ethane, 1,1-difluoro-	11.40	11.50	14.70 25	Creazzo, JA et al., (1993)	
000075434	Methane, dichlorofluoro-	9.43	8.50	11.20 20	Suh, KW. (1994)	
000075456	Methane, chlorodifluoro-	10.70	10.50	10.90 23	Cecchini, C. et al. (1991)	
000075616	Methane, dibromodifluoro-	7.07	6.90	0.00		
000075638	Methane, bromotrifluoro-	9.59	9.80	10.20 27	Suehla, RA. (1962)	
000075683	Ethane, 1-chloro-1,1-difluoro-	11.20	11.70	9.40 25	Wiederman, RE. et al. (1991)	
000075694	Methane, trichlorofluoro-	8.01	7.70	7.80 23	Cecchini, C. et al. (1991)	

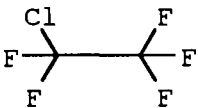
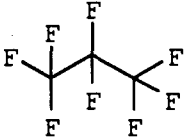
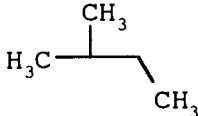
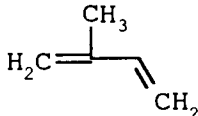
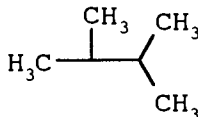
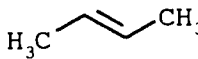
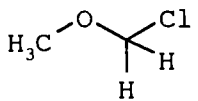
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000075718	Methane, dichlorodifluoro-	9.88	9.60	9.90 30	Wiederman, RE. et al. (1991)	
000075763	Tetramethyl silane	15.50	0.00	0.00		
000075832	Butane, 2,2-dimethyl-	14.00	13.20	0.00		
10 000075887	Ethane, 2-chloro-1,1,1-trifluoro-	9.00	0.00	0.00		
000076131	Ethane, 1,1,2-trichloro-1,2,2-trifluoro-	8.48	8.80	7.31 27	Krauss, R. and Stephan, K. (1969)	
000076142	Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-	9.93	10.20	10.25 27	Krauss, R. and Stephan, K. (1969)	

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000076153	Ethane, chloropentafluoro-	11.70	14.90	0.00		
000076197	Propane, octafluoro-	11.70	11.60	0.00		
000078784	Butane, 2-methyl-	15.00	14.80	13.00 20	Missenard, FA. (1966)	
000078795	1,3-Butadiene, 2-methyl-	13.50	14.40	0.00		
000079298	Butane, 2,3-dimethyl-	13.70	12.40	0.00		
000107017	2-Butene	14.50	13.50	0.00		
000107302	Methane, chloromethoxy-	8.84	0.00	0.00		




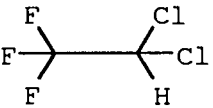
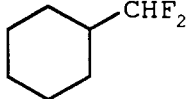
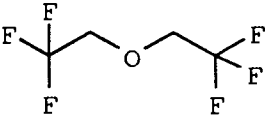
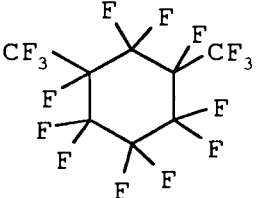
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Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000109660	Pentane	14.20	14.80	0.00		
000109671	1-Pentene	13.20	13.60	0.00		
000109682	2-Pentene	12.70	0.00	0.00		
000109875	Dimethoxymethane	14.90	0.00	0.00		
000115253	Cyclobutane, octafluoro-	11.60	10.00	12.48 27	Krauss, R. and Stephan, K. (1969)	
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-	10.90	10.47	0.00		
000124732	Ethane, 1,2-dibromo-1,1,2,2-tetrafluoro-	6.63	5.80	0.00		

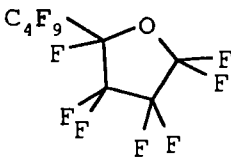
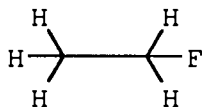
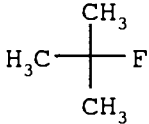
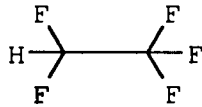
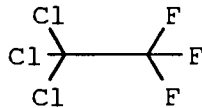
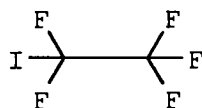
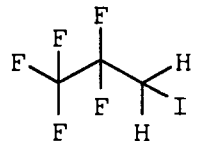
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000142290	Cyclopentene	12.10	10.80	0.00		
000287230	Cyclobutane	15.90	14.80	12.40 0	Missenard, FA. (1966)	
000287923	Cyclopentane	14.00	12.10	11.00 20	Missenard, FA. (1966)	
000306832	Ethane, 2,2-dichloro-1,1,1-trifluoro-	8.74	0.00	9.30 23	Cecchini, C. et al. (1991)	
000329293		11.90	0.00	0.00		
000333368	Bis-2,2,2-trifluoroethyl ether	9.93	0.00	0.00		
000335273	Cyclohexane, 1,1,2,2,3,3,4,4,5,5,6-decafluoro-4,6-bis(trifluoromethyl)-	9.42	0.00	0.00		

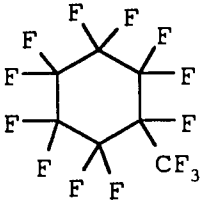
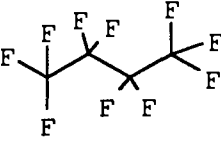
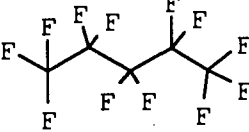
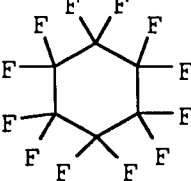
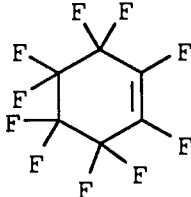
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Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000335364	Furan, 2,2,3,3,4,4,5-heptafluorotetrahydro-5-(nonafluorobutyl)-	8.45	0.00	0.00		
000353366	Ethane, fluoro-	13.90	13.80	0.00		
000353617	Propane, 2-fluoro-2-methyl-	13.80	0.00	0.00		
000354336	Ethane, pentafluoro-	11.00	10.90	14.30 23	Cecchini, C. et al. (1991)	
000354585	Ethane, 1,1,1-trichloro-2,2,2-trifluoro-	10.40	0.00	7.20 20	Suh, KW. (1994)	
000354643	Ethane, pentafluoroiodo-	8.30	0.00	0.00		
000354698	Propane, 1,1,1,2,2-pentafluoro-3-iodo-	5.80	0.00	0.00		

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000355022	Cyclohexane, undecafluoro(trifluoromethyl)-	9.89	0.00	0.00		
000355259	Butane, decafluoro-	10.40	10.30	0.00		
000355420	Hexane, tetradecafluoro-	8.40	0.00	0.00		
000355680		9.73	0.00	0.00		
000355759		8.95	0.00	0.00		

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference
000356707		8.99	0.00	0.00	
000359580		9.86	0.00	0.00	
000360521	2-Propanone, 1,1,3,3-tetrafluoro	9.63	0.00	0.00	
000360576		10.60	0.00	0.00	
000371904		11.90	0.00	0.00	
000372907	1,4-Difluorobutane	13.00	0.00	0.00	

Structure

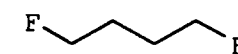
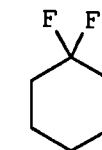
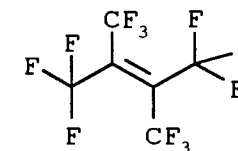
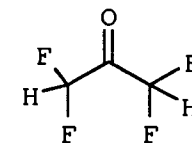
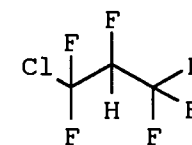
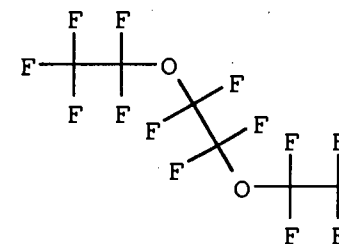
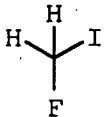
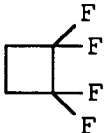
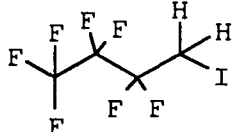
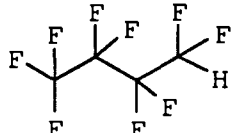
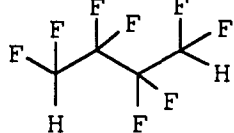
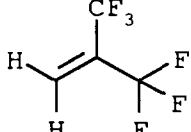
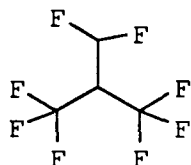
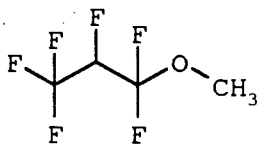
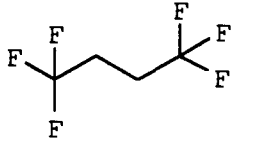
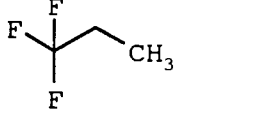
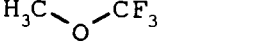
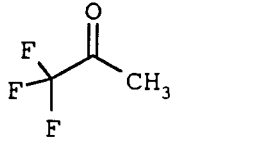
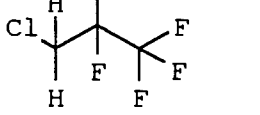
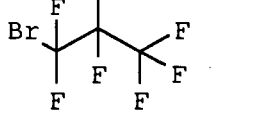


Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000373535	Methane, iodofluoro-	5.11	0.00	0.00		
000374129	1,1,2,2-Tetrafluorocyclobutane	11.00	0.00	0.00		
000374981	Butane, 1,1,1,2,2,3,3-heptafluoro-4-iodo-	6.50	0.00	0.00		
17 000375177		9.98	0.00	0.00		
000377366		8.60	0.00	0.00		
000382105	1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-	17.00	0.00	0.00		
000382207		12.30	0.00	0.00		

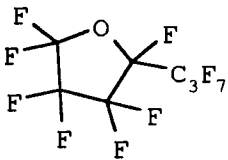
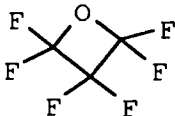
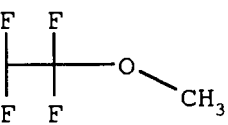
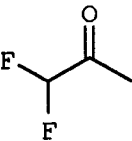
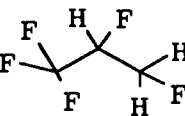
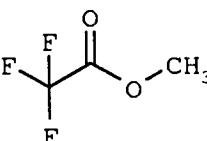
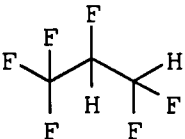
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Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000382343	1,1,2,3,3,3-Pentafluoropropyl methyl ether	9.43	0.00	0.00		
000407590	1,1,1,4,4,4-Hexafluorobutane	10.10	0.00	9.50 20	Ball, EE. and Lamberts, WM. (1993)	
000421078	Propane, 1,1,1-trifluoro-	11.00	0.00	0.00		
000421147	Trifluoromethyl methyl ether	13.70	0.00	0.00		
000421501	2-Propanone, 1,1,1-trifluoro	12.00	0.00	0.00		
000422026		9.38	0.00	0.00		
000422855	Propane, 1-bromo-1,1,2,2,3,3,3-heptafluoro-	7.19	0.00	0.00		

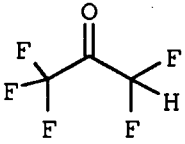
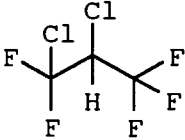
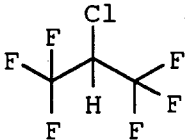
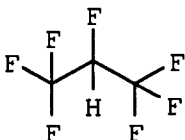
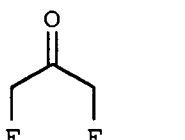
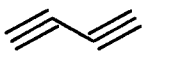
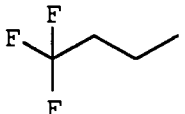
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Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000423223		9.46	0.00	0.00		
000425821	1,1,2,2,3,3-Hexafluorooxetane	13.70	0.00	0.00		
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane	12.00	0.00	0.00		
61 000431050	1,1-Difluoroacetone	14.80	0.00	0.00		
000431312	1,1,1,2,3-Pentafluoropropane	8.92	0.00	19.20 44	Knopeck, GM. et al. (1993)	
000431470	Methyl trifluoroacetate	11.00	0.00	0.00		
000431630	1,1,1,2,3,3-Hexafluoropropane	10.20	0.00	0.00		

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000431710	2-Propanone, 1,1,1,3,3-pentafluoro	9.56	0.00	0.00		
000431867		8.77	0.00	0.00		
000431878		10.00	0.00	0.00		
000431890	1,1,1,2,3,3,3-Heptafluoropropane	19.10	0.00	0.00		
000453145	1,3-Difluoroacetone	12.00	0.00	0.00		
000460128	1,3-Butadiyne	14.20	0.00	0.00		
000460344	1,1,1-Trifluorobutane	12.00	0.00	0.00		

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference
000460435	1-Methoxy-2,2,2-trifluoroethane	12.50	0.00	11.84 25	Smith, ND. (1993)
000460731	1,1,1,3,3-Pentafluoropropane	9.39	0.00	0.00	
000461632	Difluoromethyl fluoromethyl ether	10.30	0.00	0.00	
000462555		10.30	0.00	0.00	
000503173	2-Butyne	12.50	14.20	0.00	
000503300	Trimethylene oxide	13.80	0.00	0.00	
000504609	1,3-Pentadiene	12.10	0.00	0.00	

Structure

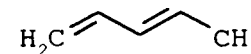
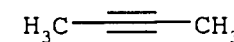
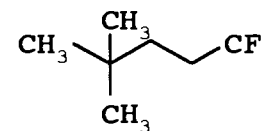
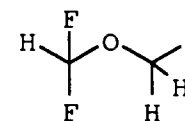
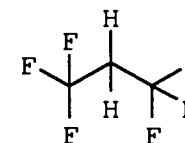
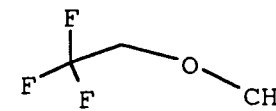
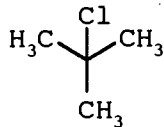
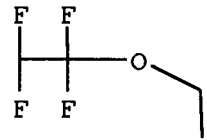
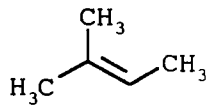
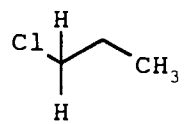

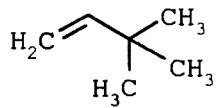
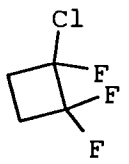
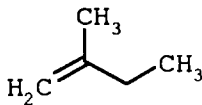

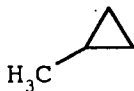

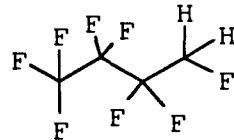
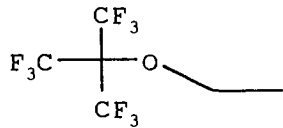
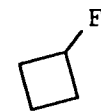


Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000507200	Propane, 2-chloro-2-methyl-	11.70	11.50	0.00		
000512516	1,1,2,2-Tetrafluoroethyl ethyl ether	12.20	0.00	0.00		
000513359	2-Butene, 2-methyl-	13.20	14.10	0.00		
000540545	Propane, 1-chloro-	9.79	10.80	8.50 0	Missenard, FA. (1966)	
000542927	1,3-Cyclopentadiene	11.70	13.10	0.00		
000558372	1-Butene, 3,3-dimethyl-	13.00	12.40	0.00		
000558612		10.20	0.00	0.00		

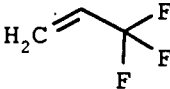
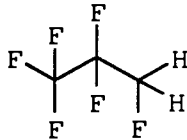
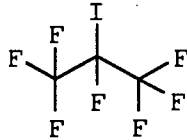
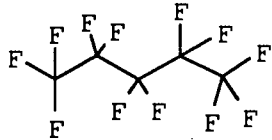
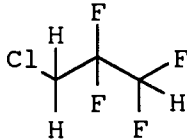
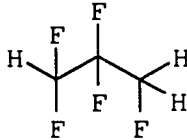
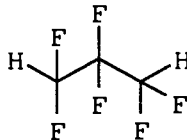
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000563462	1-Butene, 2-methyl-	13.60	12.90	0.00		
000591935	1,4-Pentadiene	12.60	12.60	0.00		
000594116	Cyclopropane, methyl-	13.50	0.00	0.00		
000627190	1-Pentyne	13.40	13.60	0.00		
000662351		9.33	0.00	0.00		
000665167		11.10	0.00	0.00		
000666160	Fluorocyclobutane	13.50	0.00	0.00		

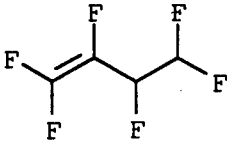
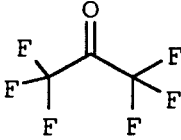
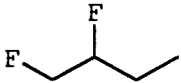
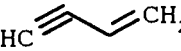
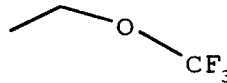
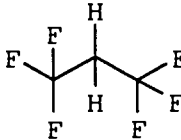
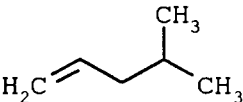
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Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000677214	1-Propene, 3,3,3-trifluoro-	10.90	0.00	0.00		
000677565	1,1,1,2,2,3-Hexafluoropropane	10.00	0.00	0.00		
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-	8.54	0.00	0.00		
24 000678262	Pentane, dodecafluoro-	6.60	0.00	0.00		
000679856		8.29	0.00	0.00		
000679867	1,1,2,2,3-Pentafluoropropane	8.81	0.00	15.90 44	Knopeck, GM et al. (1993)	
000680002	1,1,2,2,3,3-Hexafluoropropane	9.27	0.00	0.00		

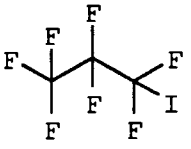
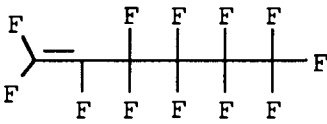
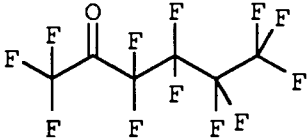
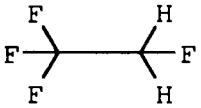
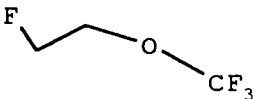
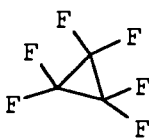
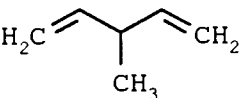
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000680546	1,1,2,3,4,4-Hexafluoro-1-butene	11.00	0.00	0.00		
000684162	2-Propanone, hexafluoro	13.70	0.00	0.00		
000686657	1,2-Difluorobutane	13.00	0.00	0.00		
000689974	1-Buten-3-yne	13.80	0.00	0.00		
000690222	Trifluoromethyl ethyl ether	12.50	0.00	0.00		
000690391	1,1,1,3,3,3-Hexafluoropropane	10.10	0.00	0.00		
000691372	1-Pentene, 4-methyl-	12.30	11.70	0.00		


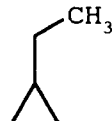
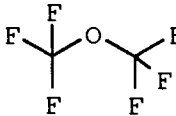
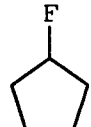
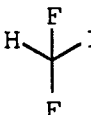
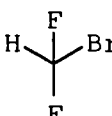
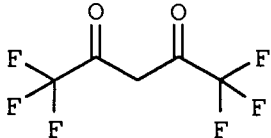
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-	8.06	0.00	0.00		
000755259		9.86	0.00	0.00		
000755271		8.68	0.00	0.00		
26 000811972	Ethane, 1,1,1,2-tetrafluoro-	9.70	9.10	14.50 20	Creazzo. JA et al. (1993)	
000819498	1-Trifluoromethoxy-2-fluoroethane	12.10	0.00	0.00		
000931919	Hexafluorocyclopropane	10.90	0.00	0.00		
001115088	1,4-Pentadiene, 3-methyl-	12.70	0.00	0.00		

A value of 0.00 indicates that no data are available

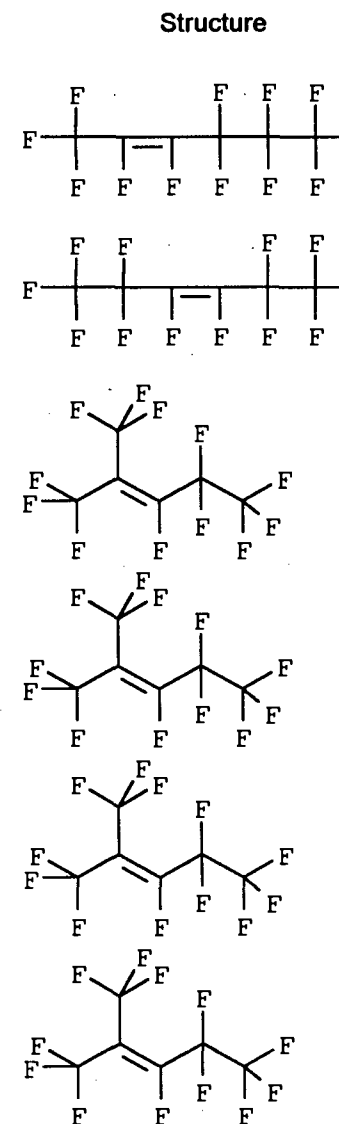
Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
001120203	1,1-Difluorocyclopentane	12.60	0.00	0.00		
001191964	Cyclopropane, ethyl-	15.60	0.00	0.00		
001479498	Trifluoromethyl ether	12.70	0.00	0.00		
001481363	Fluorocyclopentane	13.30	0.00	0.00		
001493034	Methane, iododifluoro-	6.25	0.00	0.00		
001511622	Methane, bromodifluoro-	8.97	0.00	0.00		
001522221		7.92	0.00	0.00		

A value of 0.00 indicates that no data are available

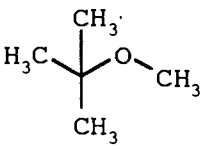
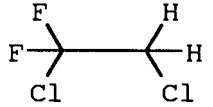
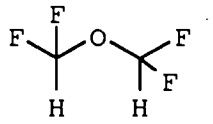
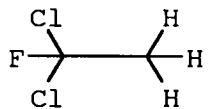
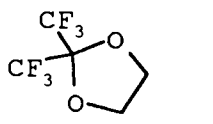
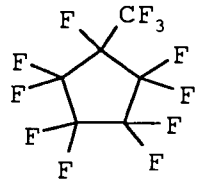
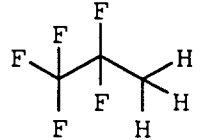
Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference
001584005		9.86	0.00	0.00	
001584027		9.86	0.00	0.00	
001584038		10.30	0.00	0.00	
28 001584038		10.30	0.00	0.00	
001584038		10.60	0.00	0.00	
001584038		10.60	0.00	0.00	



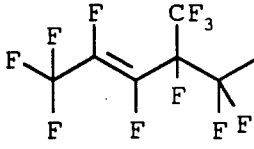
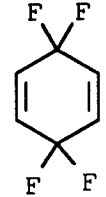
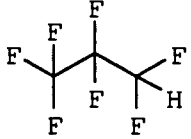
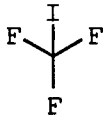
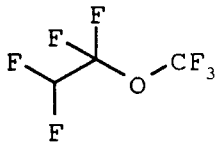
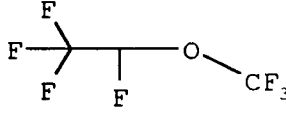
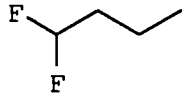
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
001634044	t-Butyl methyl ether	14.40	0.00	0.00		
001649087	Ethane, 1,2-dichloro-1,1-difluoro-	16.90	0.00	0.00		
001691174	Difluoromethyl ether	12.50	0.00	0.00		
001717006	Ethane, 1,1-dichloro-1-fluoro-	9.46	0.00	9.20 23	Cecchini, C. et al. (1991)	
001765260		11.40	0.00	0.00		
001805227	Cyclopentane, nonafluoro(trifluoromethyl)-	10.50	0.00	0.00		
001814886	1,1,1,2,2-Pentafluoropropane	11.50	0.00	0.00		


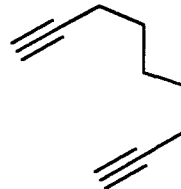
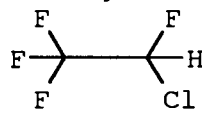
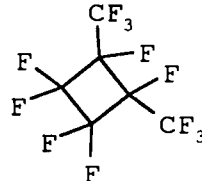
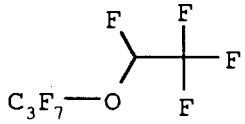
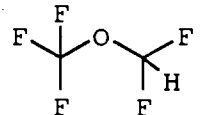
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
002070704		10.30	0.00	0.00		
002206771		10.40	0.00	0.00		
002252848	1,1,1,2,2,3,3-Heptafluoropropane	11.00	0.00	0.00		
002314978	Methane, trifluoroiodo-	8.06	0.00	0.00		
002356618		10.90	0.00	0.00		
002356629		11.40	0.00	0.00		
002358385	1,1-Difluorobutane	13.00	0.00	0.00		

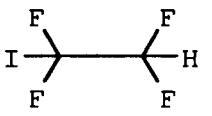
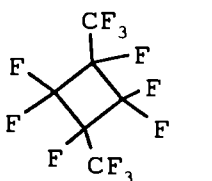
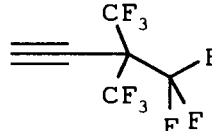
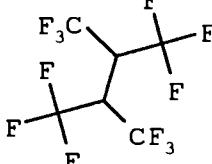
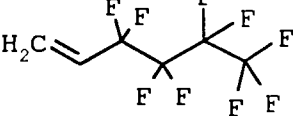
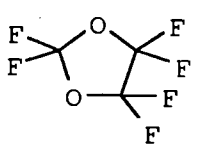
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
002366521	Butane, 1-fluoro-	12.50	0.00	0.00		
002396658	1,8-Nonadiyne	15.60	0.00	0.00		
002837890	Ethane, 2-chloro-1,1,1,2-tetrafluoro-	18.00	0.00	15.90 80	Creazzo, JA. and Hammel, HS. (1991)	
002994710	Cyclobutane, 1,1,2,2,3,3,4-hexafluoro-3,4-bis(trifluoromethyl)-	11.40	0.00	0.00		
003330152	Propane, 1,1,1,2,2,3,3-heptafluoro-3-(1,2,2,2-tetrafluoroethoxy)-	13.10	0.00	0.00		
003822682	Trifluoromethyl difluoromethyl ether	16.20	0.00	0.00		


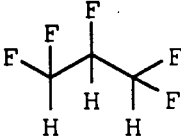
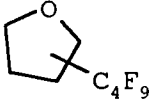
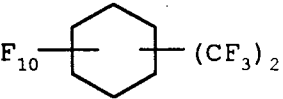
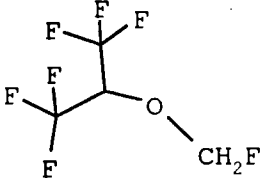
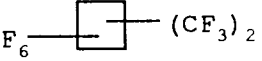
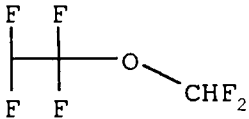
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-	7.45	0.00	0.00		
013221711	Cyclobutane, 1,1,2,3,3,4-hexafluoro-2,4-bis(trifluoromethyl)-	11.70	0.00	0.00		
014115481		12.60	0.00	0.00		
017737223		11.40	0.00	0.00		
019430934	1-Hexene, 3,3,4,4,5,5,6,6-nonafluoro-	9.78	0.00	0.00		
021297654		18.90	0.00	0.00		

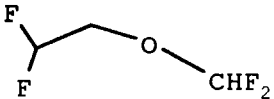
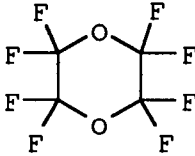
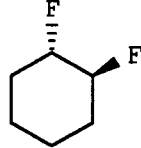
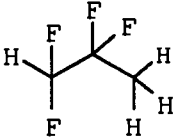
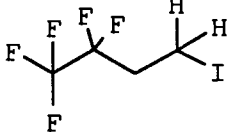
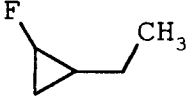
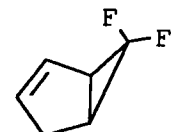
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
022669096	1,1-Difluorocyclobutane	12.80	0.00	0.00		
024270664	1,1,2,3,3-Pentafluoropropane	8.19	0.00	0.00		
026446593		19.30	0.00	0.00		
026637683		9.42	0.00	0.00		
028523866		12.20	0.00	0.00		
028677001		11.40	0.00	0.00		
032778113	1-Difluoromethoxy-1,1,2,2-tetrafluoroethane	11.50	0.00	0.00		

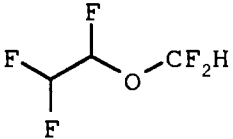
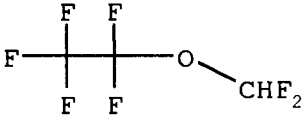
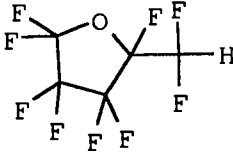
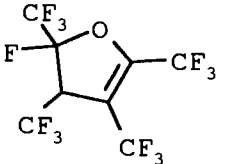
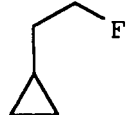
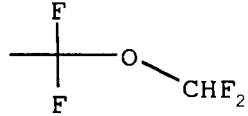
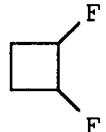
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
032778168	1-Difluoromethoxy-2,2-difluoroethane	12.00	0.00	0.00		
032981229		13.90	0.00	0.00		
038706739		11.90	0.00	0.00		
34 040723635	1,1,2,2-Tetrafluoropropane	10.70	0.00	0.00		
040723806	Butane, 1,1,1,2,2-pentafluoro-4-iodo-	6.63	0.00	0.00		
050422769	1-Fluoro-2-ethylcyclopropane	14.50	0.00	0.00		
054264992		12.80	0.00	0.00		

A value of 0.00 indicates that no data are available

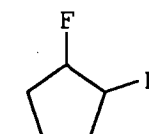
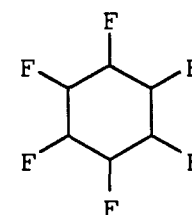
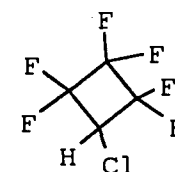
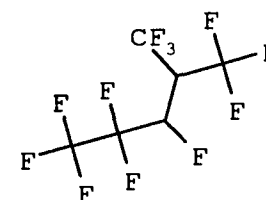
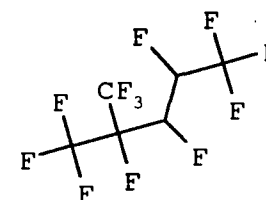
Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
056281926	1-Difluoromethoxy-1,2,2-trifluoroethane	11.70	0.00	0.00		
057041675		11.30	0.00	0.00		
065601685		11.10	0.00	0.00		
068217469		8.60	0.00	0.00		
069750681	2-Fluoroethylcyclopropane	14.50	0.00	0.00		
069948294	1-Difluoromethoxy-1,1-difluoroethane	12.00	0.00	0.00		
072507858	1,2-Difluorocyclobutane	12.70	0.00	0.00		

A value of 0.00 indicates that no data are available

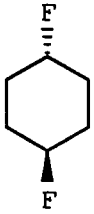
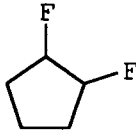
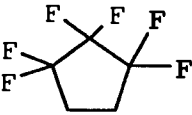

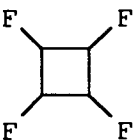
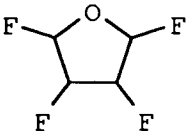
Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference
085720781		10.90	0.00	0.00	
090278005		10.90	0.00	0.00	
1	1-Chloro-2,2,3,3,4,4-hexafluorocyclobutane	14.60	0.00	0.00	
111		8.74	0.00	0.00	
113742908	1,2-Difluorocyclopentane	12.50	0.00	0.00	



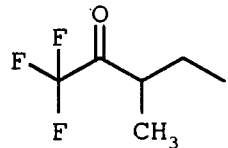
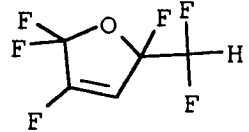
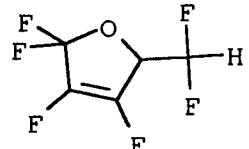
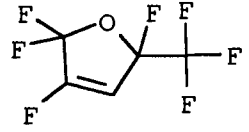
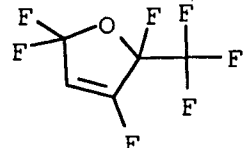
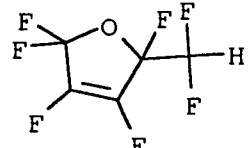
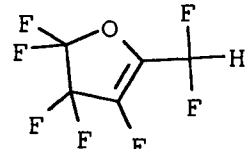
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
116199292		11.90	0.00	0.00		
123		12.50	0.00	0.00		
123768183	1,1,2,2,3,3-Hexafluorocyclopentane	11.20	0.00	0.00		
123812806	3-Fluorocyclobutene	12.50	0.00	0.00		
129362976	1,2,3,4-Tetrafluorocyclobutane	11.40	0.00	0.00		
133360006	2,3,4,5-Tetrafluorotetrahydrofuran	14.80	0.00	0.00		

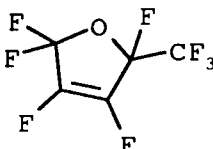
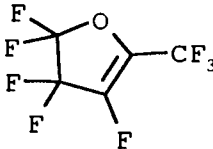
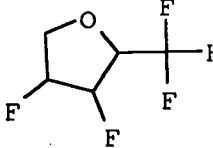
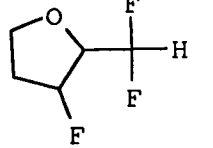
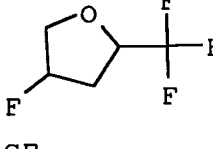
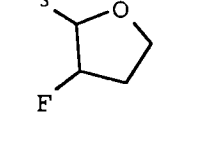
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
134166497		11.00	0.00	0.00		
135617435		10.80	0.00	0.00		
135617446		12.00	0.00	0.00		
38 135617457		10.50	0.00	0.00		
135617468		10.50	0.00	0.00		
135617479		10.10	0.00	0.00		
135617480		10.30	0.00	0.00		

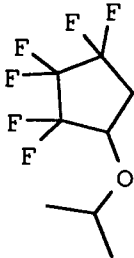
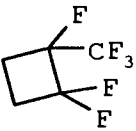
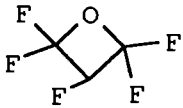
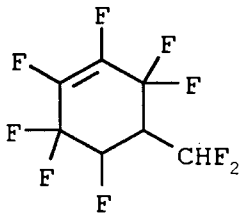
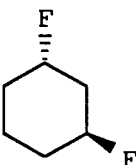
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
135617491		10.00	0.00	0.00		
135617504		10.00	0.00	0.00		
135617571		12.10	0.00	0.00		
39 135617640		12.50	0.00	0.00		
135617662		12.50	0.00	0.00		
135617673		12.10	0.00	0.00		

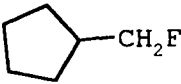
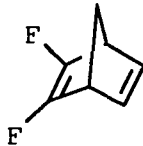
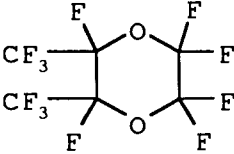
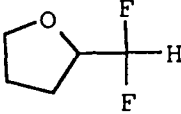
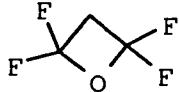
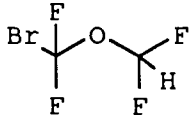
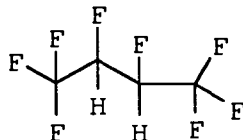
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
135947169		9.17	0.00	0.00		
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane	12.10	0.00	0.00		
144109035	1,1,2,2,3-Pentafluorooxetane	13.00	0.00	0.00		
144963699		9.62	0.00	0.00		
145354887		11.90	0.00	0.00		

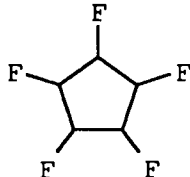
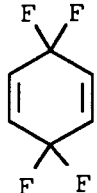
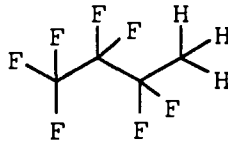
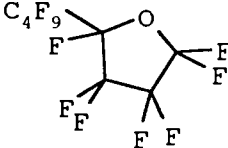
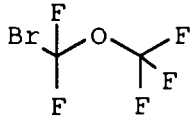
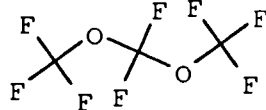
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
145866235		13.70	0.00	0.00		
146229289		11.70	0.00	0.00		
146780203		9.77	0.00	0.00		
41 147356670		13.10	0.00	0.00		
154330402	1,1,3,3-Tetrafluorooxetane	12.20	0.00	0.00		
19	Bromodifluoromethyl difluoromethyl ether	11.30	0.00	0.00		
22	1,1,1,2,3,4,4,4-Octafluorobutane	10.20	0.00	0.00		

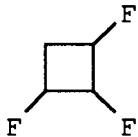
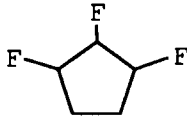
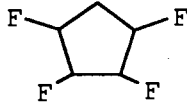
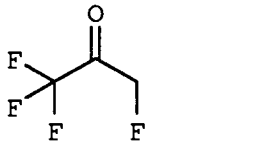

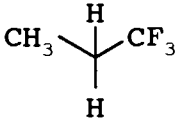
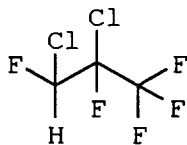
A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
222		9.51	0.00	0.00		
234		12.30	0.00	0.00		
25	1,1,1,2,2,3,3-Heptafluorobutane	10.30	0.00	0.00		
345		11.00	0.00	0.00		
39	Bromodifluoromethyl trifluoromethyl ether	14.60	0.00	0.00		
40	Bis(trifluoromethoxy)difluoromethane	15.20	0.00	0.00		

A value of 0.00 indicates that no data are available

Table 1. Experimental and Estimated Vapor Thermal Conductivities in mW/(m K) (continued)

CAS Registry Number	Name	Estimated	Daubert and Danner (1989)	Literature Temp	Reference	Structure
6104	1,2,3-Trifluorocyclobutane	12.20	0.00	0.00		
6108	1,2,3-Trifluorocyclopentane	12.00	0.00	0.00		
6109	1,2,3,4-Tetrafluorocyclopentane	12.00	0.00	0.00		
6112	1,1,1,3-Tetrafluoroacetone	11.00	0.00	0.00		
6119	Trifluoromethoxymethoxymethane	12.80	0.00	0.00		
6330		12.90	0.00	0.00		
64	1,2-Dichloro-1,2,3,3,3-pentafluoropropane	8.73	0.00	0.00		

A value of 0.00 indicates that no data are available

Experimental

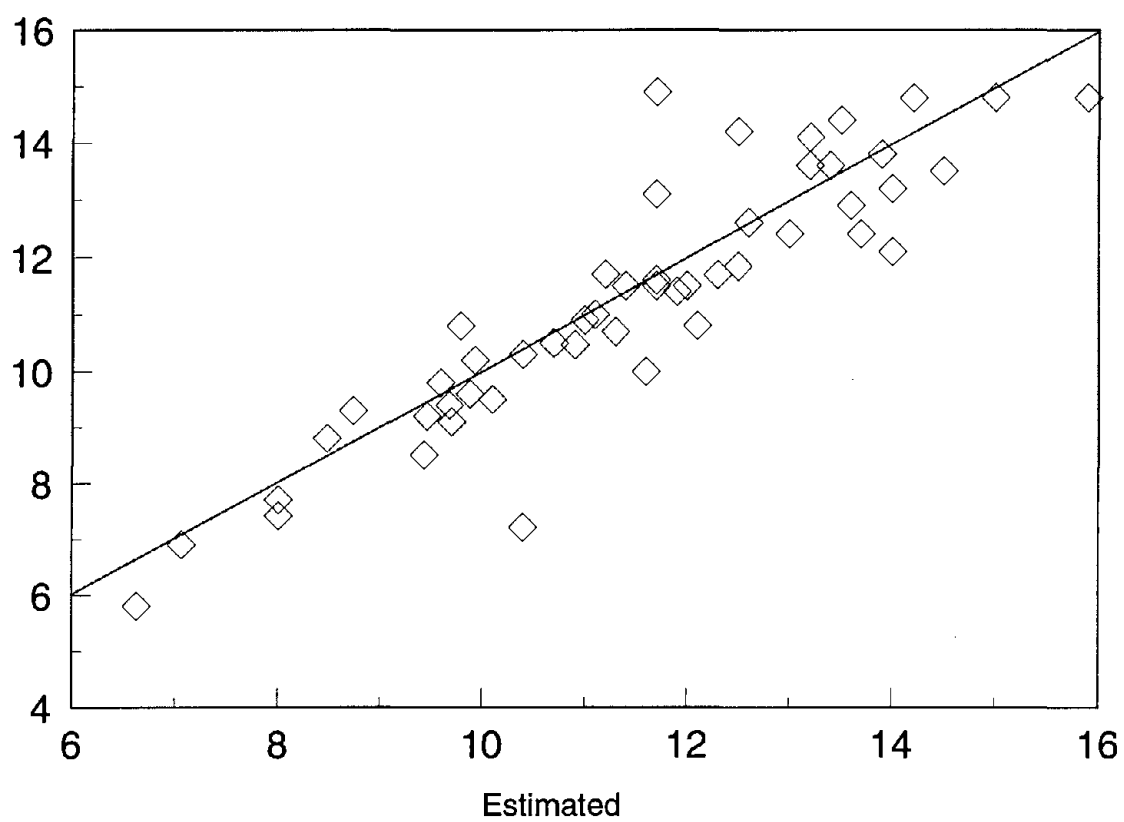


Figure 2. Estimated vs. Experimental Vapor Thermal Conductivities in mW/(m K)

mW/(m K) were very close to the experimental values and that the greatest deviation occurred in the high-range estimates. The majority of compounds considered in phase 2 of this task had thermal conductivities in the 8 to 13 mW/(m K) range.

Critical Temperature and Pressure

To perform the vapor thermal conductivity estimates, critical temperature (T_c) and pressure (P_c) needed to be estimated first if experimental values could not be found in the open literature. These were obtained by Joback's method (Joback, KG., 1982; Reid, RC. et al., 1987). Estimation of these values also required a boiling point that could be obtained, as required, from Joback's method (Joback, KG., 1982). This method was advantageous as the fragment groups for the Joback method are the same for the normal boiling point (T_b), T_c , and P_c ; however, ΔT_c and ΔP_c need to be summed for estimating the critical temperature and critical pressure, respectively. The critical temperature (T_c in K) and critical pressure (P_c in bars) are then obtained from the equations

$$T_c = T_b [0.584 + 0.965 \Sigma \Delta T_c - (\Sigma \Delta T_c)^2]^{-1}$$

and

$$P_c = (0.113 + 0.0032 n_A - \Sigma \Delta P_c)^{-2}$$

where n_A is the number of atoms in the molecule. T_b represents the normal boiling point.

For cyclic hydrocarbons, group contributions are available only for $-\text{CH}_2-$ (4.25) and $-\text{CH}=$ (3.50). Thus, there is no recommended way to estimate C for substituted cyclic hydrocarbons. In this study, we have assigned the value for $-\text{CH}_2-$ (4.25) to both $-\text{C}-$ and $-\text{CH}-$ groups in cyclic structures. However, this only makes a minor difference to the overall thermal conductivity. For example, consider fluorocyclobutane. If a value of 4.25 is assigned to the

-CH- group, then $\lambda=13.5$ mW/(m K). If the value for -CH= of 3.50 (an extreme case) is used, $\lambda=12.7$ mW/(m K). For one or two substituents, the difference is not appreciable. On the other hand, the difference between cyclohexane and perfluorocyclohexane would be very significant since these differences would be cumulative. However, the high-priority compounds on our list are relatively small, and large differences in λ arising from uncertainty in C are expected to be unlikely.

There were several other occasions where approximations were required. For example, among ethers, a group value is only given for a primary ether group; secondary and tertiary derivatives are excluded. In our study, all ethers were assigned the group value for a primary ether.

Another source of uncertainty lies in the calculation of $f(T_r)$ which takes the form

$$f(T_r) = aT_r + bT_r^2 + cT_r^3$$

where T_r is the reduced temperature and a, b, and c are fitted coefficients. Different values of the coefficients are available for (i) saturated hydrocarbons, (ii) olefins, (iii) acetylenes, (iv) naphthalenes and aromatics, (v) alcohols, (vi) aldehydes, ketones, ethers and esters, (vii) amines and nitriles, (viii) halides, and (ix) cyclic compounds. A problem arises if a compound fits into more than one category. Consider difluoromethyl fluoromethyl ether (Chemical Abstract Service (CAS) Registry number: 461-63-2). If the "halide equation" is used, then $\lambda=13.9$ mW/(m K). If the equation for ethers is applied, then $\lambda=13.3$ mW/(m K). Again, the difference is quite small if only one or two substituents are involved.

In sum, although there were many compounds that fell outside the Roy-Thodos formalism, the errors incurred by assigning values for their structurally nearest neighbors are

expected to be quite small, and are probably insignificant for our purpose of prioritizing structures for more detailed consideration.

Developing Estimation Methods for Silicon-Containing Compounds

In the course of this investigation, it became evident that tetraalkyl silicon compounds should be considered as a potential group of blowing agent substitutes. With the exception of tetramethylsilane, however, little experimental data were available on these compounds. Moreover, estimation techniques described previously did not have group constants for the silicon atom. Therefore, we set out to develop methodology for estimating the vapor thermal conductivity of tetraalkyl silicon compounds.

Roy-Thodos Constant

Thermal conductivities, critical properties, and boiling points were obtained from the literature for the fourteen silicon compounds (Si) in Table 2. Since the data set is quite small and covers a narrow range of thermal conductivity, it was impractical to derive formal equations for silicon compounds. Instead, a “perturbation” method was used. Here, experimental partial C values were first back calculated for compounds containing silicon which have known thermal conductivity values from the literature P_c , T_c , T_b , and λ values. Partial C values for the silicon groups were then obtained by subtracting out the known partial values of C for the other groups. Although there are five kinds of silicon groups (Si to SiH_4 in Table 2), the values were too close to be separated, and a single value of C of 3.23 was averaged for all the groups.

Boiling Point

Using known boiling points of compounds containing silicon groups, estimates of the contribution a silicon group makes to the normal boiling point of a compound were made using

Table 2. Properties of Silicon Compounds

	CAS #	λ	Pc	Tc	Tb	MW
Silane, dichloromethyl	75-54-7	10.27	39.5	483	315	115
Silane, tetramethyl	75-76-3	15.51	28.1	450	300	88
Silane, chlorotrimethyl	75-77-4	12.2	32.0	498	331	109
Silane, dichlorodimethyl	75-78-5	9.8	34.9	520	343	129
Silane, trichloromethyl	75-79-6	8.52	35.3	517	400	149
Silane, methyl	992-94-9	17.9	48.4	353	216	46
Silane, chloromethyl	993-00-0	12.56	41.7	442	282	81
Silane, trimethyl	993-07-7	15.23	31.9	432	280	74
Silane, chlorodimethyl	1066-35-9	11.9	36.2	472	309	95
Silane, dimethyl	1111-74-6	16.6	35.6	402	254	60
Silane, dichloro	4109-96-0	10.09	44.3	449	281	101
Silane	7803-62-5	22.8	48.4	270	161	32
Silane, trichloro	10025-78-2	7.92	41.7	479	305	135
Silane, tetrachloro	10026-04-7	8.49	35.9	507	330	170

λ - mW/(m K)

Pc - bars

Tc - K

Tb - K

the method of Stein and Brown (Stein, SE. and Brown, RL., 1994). This method attributes a contribution from each chemical group in the compound. Since values for the non-silicon groups were available, it was a simple matter to estimate and average group contribution values for the various silicon groups is 20, 13 and 22 for Si, SiH and SiH₂. Unfortunately, these averages have very high uncertainty. For example, the Si value of 20 is averaged from 8, 24, 22, 64, and -20. Only one compound with an SiH₃ value was available, and this value was -6. Given these variations, the averages for Si, SiH, and SiH₂ were re-averaged to give 18, and this figure was

used for all silicon groups. Estimated values of λ based on estimated boiling point contribution and actual values are compared in Table 3. Except for silane, the comparison is reasonably good, probably because the inclusion of a single silicon group has only a small impact on the overall boiling point, and the variations within these group values are, therefore, of relatively minor importance.

Table 3. Comparison of Estimated and Experimental Properties for Silicon Compounds

	λ est	λ exptl	Pc est	Pc exptl	Tc est	Tc exptl
Silane, dichloromethyl	7.0	10.27	45.4	39.5	490	483
Silane, tetramethyl	15.4	15.51	28.8	28.1	451	450
Silane, chlorotrimethyl	11.7	12.2	39.0	32.0	500	498
Silane, dichlorodimethyl	8.1	9.8	32.8	34.9	520	520
Silane, trichloromethyl	9.0	8.52	35.2	35.3	see text	517
Silane, methyl	13.7	17.9	42.2	48.4	354	353
Silane, chloromethyl	12.1	12.56	39.7	41.7	447	442
Silane, trimethyl	15.4	15.23	32.5	31.9	432	432
Silane, chlorodimethyl	114.0	11.9	34.8	36.2	see text	472
Silane, dimethyl	16.0	16.6	36.9	35.6	400	402
Silane, dichloro	12.0	10.09	42.8	44.3	447	449
Silane	28.3	22.8	48.8	48.4	270	270
Silane, trichloro	11.0	7.92	40.2	41.7	477	479
Silane, tetrachloro	7.6	8.49	37.8	35.9	505	507

λ est - mW/(m K)
 λ exptl - mW/(m K)
Pc est - bars
Pc exptl - bars
Tc est - K
Tc exptl - K

Critical Temperature

Calculation of group contribution values of T_c , called fragment constants for ΔT_c , was based on Joback's method and was estimated from the equation

$$T_c = T_b[0.584 + 0.965 \Sigma \Delta T_c - (\Sigma \Delta T_c)^2]^{-1}$$

There are two solutions for ΔT_c ; the higher value was well outside the typical range for ΔT_c , and the lower value was, therefore, taken. The ΔT_c value for the silicon groups was obtained after subtracting out the known ΔT_c values for all of the other groups. Values for two compounds (trichloromethylsilane and chlorodimethylsilane) were clear outliers. With their exclusion, the following fragment constants were derived:

$$\text{SiH}_4 \quad 0.0120 \quad n=1$$

$$\text{SiH}_3 \quad 0.0129 \quad n=1$$

$$\text{SiH}_2 \quad 0.0274 \quad n=3$$

$$\text{SiH} \quad 0.0301 \quad n=3$$

$$\text{Si} \quad 0.0367 \quad n=4$$

There is a consistent trend to the data, and the magnitude is within the range of similar groups. For example, the value for SiH_4 is very close to that of the fluorine group. Estimated and actual values for T_c using these and known other fragment constants along with experimental T_b values are compared in Table 3.

Critical Pressure

Critical pressures were estimated from the equation

$$P_c = (0.113 + 0.0032 n_A - \Sigma \Delta P_c)^{-2}$$

(which is based on Joback's method) and known values of P_c and n_A . The ΔP_c s ranged from -0.035 to -0.00394 and no statistical differences existed for values for the five types of groups involved, i.e., SiH_4 - Si. Hence, they were averaged to give a ΔP_c value of -0.0141 for any of these groups. Estimated and actual values for P_c using these and known other fragment constants along with experimental P_c values are compared in Table 3.

Overall Comparison

Thermal conductivities calculated with estimated values of P_c , T_c , and ΔC values for the Si group are compared to experimental measures in Table 3. For trichloromethyl and chloromethylsilane, experimental values of T_c were used for reasons described above. The comparison is good, suggesting that the estimated parameters are adequate for computing thermal conductivities of other structurally related compounds.

Task 2: Identification of Potential New Foam Blowing Agents.

The first step in this task was to develop a master list of potential foam blowing agent substitutes by developing an electronic database of chemical substances that could then be manipulated to obtain those substances that possess the most desirable physical/chemical properties. The list of potential blowing agents was obtained from the following sources:

- TSCA Inventory. Chemical compounds known to be produced commercially were identified. Searching by either molecular formula (for hydrocarbons) or chemical name (for ketones, ethers, halogen containing compounds, etc.), a master list containing thousands of potential candidates was obtained. Unacceptable candidates (e.g., aromatics) or compounds that would react with polyurethane foam feedstocks (e.g. amines, thiols, epoxides, or alcohols) were removed electronically by searching for those that contained sub-strings such as "anthracene" or "amino" in the chemical name field.
- Literature Sources. Additional rigid foam blowing agent candidates were obtained from periodicals such as Proceedings of the Polyurethane World Congress, patent literature, and pertinent journal articles discussing blowing agents or blown foams. If a chemical compound was identified in these sources as a possible blowing agent, it was included. This process allowed the inclusion of chemical compounds not known to be produced commercially as well as those being considered as blowing agents by commercial and academic research groups.

- Other Sources. A number of candidates were obtained from a wide variety of other sources including various EPA documents, encyclopedic sources, and chemical company literature.
- Reverse-Engineered Compounds. The results from Task 1 allowed us to develop some generalized trends relating changes in structure and functionality to vapor thermal conductivity. Starting with chemical compounds that possessed low vapor thermal conductivities, new functional groups were added (or subtracted), structures were modified, and substitution patterns were changed in order to obtain new blowing agent candidates. Some blowing agent candidates obtained through this process had not yet appeared in the chemical literature and, thus, were theoretical species.

The master list contained approximately 1,000 chemical substances when this process was completed.

The master list was then linked electronically with SRC's CHEMBASE[®] database of physical properties on 7,000 chemicals, PHYSPROP, and the Environmental Fate Data Bases (EFDB) (Howard, PH. et al., 1982; Howard, PH. et al., 1986), as well as other PC-based databases developed in-house to obtain basic physical/chemical properties on as many compounds as possible. This electronic search for physical/chemical properties was supplemented by obtaining melting points, boiling points, and vapor pressures, as well as other pertinent properties using encyclopedic sources including the Aldrich Catalog (Aldrich, 1994), Merck Index (Budavari, S. et al., 1989), Techniques of Chemistry - Organic Solvents (Riddick, JA. et al., 1986) and Daubert and Danner's compilation (Daubert, TE. and Danner, RP., 1989); the latter source also contained an extensive set of experimental vapor thermal conductivity data. Vapor phase thermal conductivity data were also collected from available sources with the 1991 and 1993 Proceedings of the Polyurethanes World Congress providing highly reliable data.

It was decided that it would be too resource intensive to calculate the vapor-phase thermal conductivity for this many chemicals, so the master list was trimmed based on boiling point. Boiling points are readily available and they provided a reliable method of removing undesirable compounds from the master list. For example, high boiling liquids do not make suitable blowing agents while low boiling liquids or gases may make effective blowing agents with proper equipment modifications. Known or experimental polyurethane foam blowing agents have boiling points ranging from approximately -50 °C (difluoromethane) to 50 °C (cyclopentane). If experimental boiling points were not available, they were estimated for this portion of the task using the Joback's method, as described in Task 1. The available data indicated that approximately 125 compounds on the master list had boiling points in the -60 to 60 °C range.

This initial list was reviewed and compared to compounds in the master list for which boiling points were not available. If any of these compounds in the master list had a reasonable match for structure, molecular weight, and functionality with a compound on the initial list, then it was added to the initial list. Compounds were also removed from the initial list as appropriate. For example, those with high vapor phase thermal conductivities relative to currently used foam blowing agents were removed as were those that, upon closer examination, were expected to react chemically with the polyurethane foam feedstocks (e.g., two fluorinated vinyl ethers were removed from further consideration at this time because they were expected to react with the feedstocks used in polyurethane foam production).

Additions to the initial list were made to expand the universe of potential blowing agents for consideration. Unlike the compounds considered previously, these new additions were not known to be produced commercially. This list was obtained by searches of Chemical Abstracts, the chemical literature, as well as other sources for compounds of an appropriate molecular

formula and/or structure that may possess the requisite physical/chemical properties at room temperature to act as blowing agents. Reverse-engineered compounds were also considered. Most of the compounds added in this exercise were fluorinated although also included were some interesting chemical classes including furans, dioxanes, silanes, pyrans, morpholines, and perfluorinated tertiary amines.

The next step was to fill any remaining data gaps for the compounds in the initial list of potential blowing agent candidates. Physical/chemical property estimations were completed. In order to estimate boiling points and vapor thermal conductivities, a new methodology was developed, as described earlier in this report. Unfortunately, vapor thermal conductivity and boiling point estimations could not be performed for an interesting class of potential blowing agents, the perfluorinated amines, because appropriate group fragments were not available for Joback's vapor thermal conductivity estimation method and they could not be derived as experimental values on similar compounds were not available.

To further limit the initial list of potential blowing agents before the ranking exercise was performed, all chlorine containing compounds were removed from further consideration since they were likely to have some ozone depletion potential. The initial presence of chlorine containing compounds was important, however, in determining the reliability of the thermal conductivity estimation methods.

Ranking the List

At a Society of the Plastics Industry (SPI) Polyurethane Division meeting on third generation blowing agents held on March 24, 1994, at Miles Inc., round-table discussions between representatives of industry, the EPA, and SRC were held to determine the most

important criteria for determining if a chemical candidate would reasonably be expected to perform as a blowing agent for polyurethane foams. The four most important criteria were concluded to be molecular weight, boiling point, vapor thermal conductivity, and global warming potential (GWP). With these criteria identified, the list of potential rigid foam blowing agent substitutes was ordered to identify the most promising alternatives. This ordering process was based on the following:



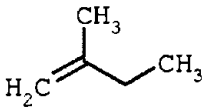

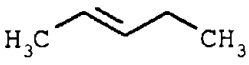


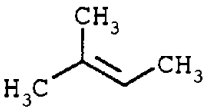
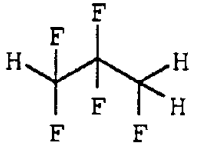
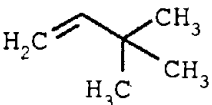
- Boiling point. According to industrial representatives present at the meeting, the best substitute blowing agent would be one that has a boiling point as close as possible to that of CFC 11 (23.8 °C), as this would reduce retro-fitting costs. For the ranking exercise, the absolute value of the difference between 23.8 °C and the boiling point of the potential blowing agent substitute was used. Thus, $\Delta BP = |BP_{CFC11} - BP_{substitute}|$. The compound with the smallest ΔBP was ranked number 1 while that with the largest was ranked number 90. For chemicals whose experimental boiling point could not be located, the boiling point was initially estimated using the method of Joback. During the later stages of this project, we had just completed work on a new product in our suite of estimation programs that estimated boiling points based on recent work by Stein and Brown (Stein, SE. and Brown, RL., 1994). Joback's method for estimating boiling point used a set of 41 groups while that of Stein and Brown used 85 groups. Based on 6,584 diverse organic compounds with experimental boiling points, the Stein and Brown method has a 3.2% average error that corresponds to an absolute error of 15.5 °C. SRC's computer estimation program is based on Stein and Brown's method and it was used to estimate boiling points for all blowing agent candidates that did not have experimental values available for the ordering exercise. However, because of resource constraints, the estimated vapor thermal conductivities were not recalculated with the more accurate boiling points.
- Molecular weight. The molecular weight also addresses the economics of using a substance as a blowing agent since the higher the value, the more costly the compound on a price by weight basis. Allied-Signal researchers (Decaire, BR. et al., 1992) used an arbitrary molecular weight cut-off of 180 in their evaluation of new blowing agents, and we removed all compounds with a molecular weight >182 from our ranking list, with the exception of perfluoroalkyl iodides (which, as described below, have some interesting

properties and, we believe, should not be eliminated solely because of their potential cost of use). For the molecular weight ranking, the lowest molecular weight compound was ranked number 1.

- **GWP.** A determination of a compound's GWP is important because it addresses the issues associated with greenhouse gases. Rigorous estimations of global warming potential are extremely complex and time consuming. The GWP is dependent, in part, on a compound's atmospheric lifetime, and, in part, on the infra red (IR) absorption strength in the 800-1200 cm^{-1} region (Wuebbles, DJ., and Edmonds, J., 1991). For a first order approximation, compounds which have a short atmospheric lifetime are the ones most likely to have a low GWP. An organic compound's atmospheric lifetime can be estimated from the rate of its vapor-phase reaction with hydroxyl radicals. The more rapid the rate constant for this reaction, the less likely the compound will contribute to global warming. Hydroxyl radical reaction rates are available experimentally or can be estimated using the method of Atkinson (Meylan, WM. and Howard, PH., 1993). For ordering the list by GWP, experimental rate constants for vapor-phase hydroxyl radical reactions were obtained from SRC's EFDB (Howard, PH. et al., 1982; Howard, PH. et al., 1986), literature reviews (Atkinson, R., 1985; Atkinson, R., 1994) or estimated using our Atmospheric Oxidation Potential (AOP) computer program which is based on Atkinson's method. The compound with the highest hydroxyl radical reaction rate constant was assigned number 1.
- **Vapor thermal conductivity.** Vapor thermal conductivity values were collected or estimated as described earlier. For thermal conductivity, the compound with the lowest value was ranked number 1.

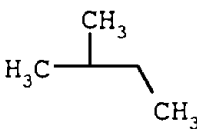
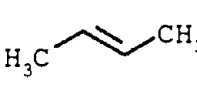

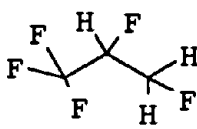
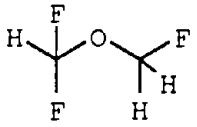
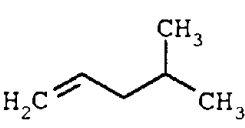
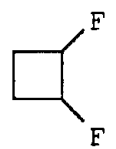

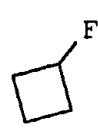
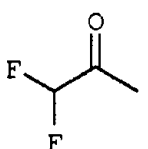
After the ranks for each of the four areas were assigned, they were added together to establish an overall score. This methodology weighs all four criteria equally. The results of this ranking exercise are provided in Table 4 in order of overall rank (left column). The column

Table 4. Final Ranking of Blowing Agent Candidates

000142290	Cyclopentene								
1	Rank:	BP : 44.00 exp 52	GWP : 65.50 2	MW : 68.12 9	TC : 10.80 24	exp			
000591935	1,4-Pentadiene								
2	Rank:	BP : 26.00 exp 7	GWP : 53.30 8	MW : 68.12 10	TC : 12.60 68	exp			
000563462	1-Butene, 2-methyl-								
3	Rank:	BP : 31.00 exp 20	GWP : 60.70 3	MW : 70.14 13	TC : 12.90 76	exp			
123812806	3-Fluorocyclobutene								
4	Rank:	BP : 32.67 25	GWP : 56.26 6	MW : 72.00 17	TC : 12.50 67				
000109682	2-Pentene								
5	Rank:	BP : 37.00 exp 34	GWP : 57.27 4	MW : 70.14 12	TC : 12.70 70	exp			
000109671	1-Pentene								
6	Rank:	BP : 29.90 exp 18	GWP : 31.40 10	MW : 70.14 14	TC : 13.60 86	exp			
002366521	Butane, 1-fluoro-								
7	Rank:	BP : 32.50 23	GWP : 2.29 28	MW : 76.11 22	TC : 12.50 65				
000513359	2-Butene, 2-methyl-								
8	Rank:	BP : 35.00 exp 30	GWP : 86.90 1	MW : 70.14 15	TC : 14.10 93	exp			
000679867	1,1,2,2,3-Pentafluoropropane								
9	Rank:	BP : 25.10 exp 5	GWP : 0.13 59	MW : 134.05 69	TC : 8.81 9	exp			
000558372	1-Butene, 3,3-dimethyl-								
10	Rank:	BP : 41.00 exp 44	GWP : 28.50 12	MW : 84.16 26	TC : 12.40 61	exp			

BP = Boiling point in degrees C exp = experimental value
TC = Vapor thermal conductivity in mW/(m · K)
MW = Molecular weight
GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

Table 4. Final Ranking of Blowing Agent Candidates (continued)

000078784	Butane, 2-methyl-								
11	BP : 28.00 exp	GWP : 3.90	MW : 72.15	TC : 14.80	exp				
	Rank: 11	21	18	97					
000107017	2-Butene								
12	BP : 1.00 exp	GWP : 56.39	MW : 56.11	TC : 13.50					
	Rank: 58	5	3	83					
000287923	Cyclopentane								
13	BP : 50.00 exp	GWP : 5.16	MW : 70.14	TC : 12.10	exp				
	Rank: 68	18	11	54					
000431312	1,1,1,2,3-Pentafluoropropane								
14	BP : 22.70	GWP : 0.06	MW : 134.05	TC : 8.92					
	Rank: 4	70	70	10					
000461632	Difluoromethyl fluoromethyl ether								
15	BP : 29.90	GWP : 0.05	MW : 100.04	TC : 10.30					
	Rank: 17	73	43	21					
000691372	1-Pentene, 4-methyl-								
16	BP : 53.00 exp	GWP : 30.11	MW : 84.16	TC : 11.70	exp				
	Rank: 76	11	25	43					
072507858	1,2-Difluorocyclobutane								
17	BP : 24.07	GWP : 0.33	MW : 92.00	TC : 12.70					
	Rank: 1	49	34	73					
000372907	1,4-Difluorobutane								
18	BP : 28.82	GWP : 2.05	MW : 94.11	TC : 13.00					
	Rank: 14	30	38	77					
000666160	Fluorocyclobutane								
19	BP : 29.19	GWP : 0.64	MW : 74.00	TC : 13.50					
	Rank: 15	43	20	85					
000431050	1,1-Difluoroacetone								
20	BP : 34.13	GWP : 0.07	MW : 94.00	TC : 11.00					
	Rank: 28	68	36	32					

BP = Boiling point in degrees C

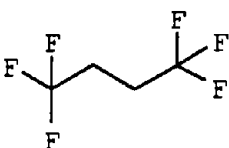
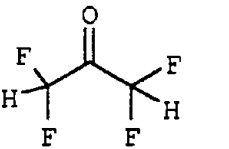
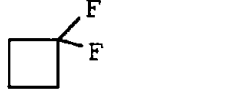

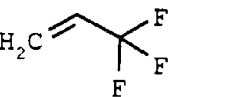

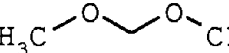
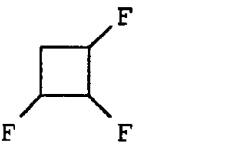
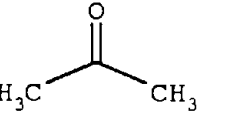
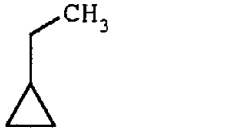
TC = Vapor thermal conductivity in mW/(m - K)

MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

exp = experimental value

Table 4. Final Ranking of Blowing Agent Candidates (continued)

000407590	1,1,1,4,4,4-Hexafluorobutane									
21	BP : 24.90 exp	GWP : 0.16	MW : 166.07	TC : 9.50						
	Rank: 3	56	92	14						
000360521	2-Propanone, 1,1,3,3-tetrafluoro									
22	BP : 23.31	GWP : 0.01	MW : 130.04	TC : 9.63						
	Rank: 2	87	62	16						
022669096	1,1-Difluorocyclobutane									
23	BP : 17.69	GWP : 0.92	MW : 92.00	TC : 12.80						
	Rank: 19	40	35	74						
000109660	Pentane									
24	BP : 36.10 exp	GWP : 3.94	MW : 72.15	TC : 14.80 exp						
	Rank: 33	20	19	98						
000677214	1-Propene, 3,3,3-trifluoro-									
25	BP : -18.00 exp	GWP : 26.30	MW : 96.05	TC : 10.90						
	Rank: 90	13	41	27						
000287230	Cyclobutane									
26	BP : 12.50 exp	GWP : 1.20	MW : 56.11	TC : 14.80 exp						
	Rank: 31	36	5	99						
6119	Trifluoromethoxymethoxymethane									
27	BP : 29.52	GWP : 3.43	MW : 130.00	TC : 12.80						
	Rank: 16	24	61	75						
6104	1,2,3-Trifluorocyclobutane									
28	BP : 18.92	GWP : 0.13	MW : 110.00	TC : 12.20						
	Rank: 12	58	48	59						
000067641	Acetone									
29	BP : 56.00 exp	GWP : 0.23	MW : 58.08	TC : 11.25 exp						
	Rank: 81	53	7	38						
001191964	Cyclopropane, ethyl-									
30	BP : 34.50	GWP : 1.38	MW : 70.14	TC : 15.60						
	Rank: 29	32	16	103						

BP = Boiling point in degrees C

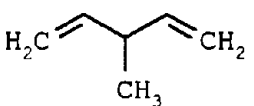
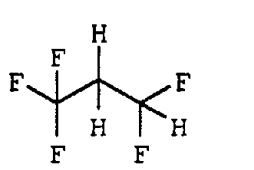
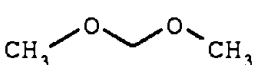
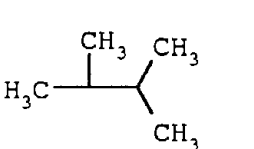

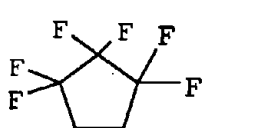
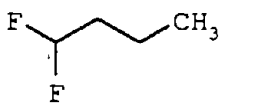

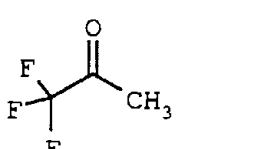
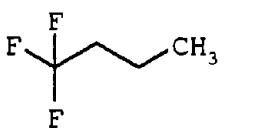
exp = experimental value

TC = Vapor thermal conductivity in mW/(m - K)

MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

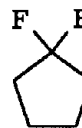
Table 4. Final Ranking of Blowing Agent Candidates (continued)

001115088	1,4-Pentadiene, 3-methyl-									
31	BP : 55.00 exp	GWP : 54.62	MW : 82.15	TC : 12.70						
	Rank: 79	7	24	71						
000460731	1,1,1,3,3-Pentafluoropropane									
32	BP : 15.30 exp	GWP : 0.03	MW : 134.05	TC : 9.39						
	Rank: 21	77	71	13						
000109875	Dimethoxymethane									
33	BP : 41.00 exp	GWP : 6.87	MW : 76.00	TC : 14.90						
	Rank: 45	16	21	101						
000079298	Butane, 2,3-dimethyl-									
34	BP : 58.00 exp	GWP : 6.20	MW : 86.18	TC : 12.40 exp						
	Rank: 83	17	27	60						
000594116	Cyclopropane, methyl-									
35	BP : 4.00	GWP : 0.28	MW : 56.11	TC : 13.50						
	Rank: 51	50	4	84						
123768183	1,1,2,2,3,3-Hexafluorocyclopentane									
36	BP : 13.58	GWP : 2.23	MW : 178.00	TC : 11.20						
	Rank: 27	29	97	37						
002358385	1,1-Difluorobutane									
37	BP : 8.56	GWP : 1.40	MW : 94.11	TC : 13.00						
	Rank: 40	31	40	79						
000503300	Trimethylene oxide									
38	BP : 50.00 exp	GWP : 3.73	MW : 58.00	TC : 13.80						
	Rank: 70	22	6	92						
000421501	2-Propanone, 1,1,1-trifluoro									
39	BP : 26.21	GWP : 0.02	MW : 112.05	TC : 12.00						
	Rank: 9	86	50	46						
000460344	1,1,1-Trifluorobutane									
40	BP : 0.38	GWP : 1.35	MW : 112.00	TC : 12.00						
	Rank: 60	33	49	49						

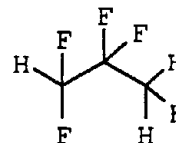
BP = Boiling point in degrees C
 TC = Vapor thermal conductivity in mW/(m · K)
 MW = Molecular weight
 GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec
 exp = experimental value

Table 4. Final Ranking of Blowing Agent Candidates (continued)

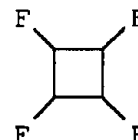
001120203 1,1-Difluorocyclopentane
 41 BP : 46.57 GWP : 4.46 MW : 106.00 TC : 12.60
 Rank: 57 19 47 69



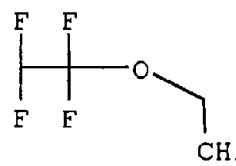
040723635 1,1,2,2-Tetrafluoropropane
 42 BP : -1.60 exp GWP : 0.21 MW : 116.06 TC : 10.70
 Rank: 65 54 53 23



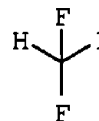
129362976 1,2,3,4-Tetrafluorocyclobutane
 43 BP : 13.74 GWP : 0.05 MW : 128.00 TC : 11.40
 Rank: 26 72 58 39



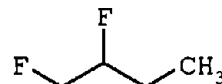
000512516 1,1,2,2-Tetrafluoroethyl ethyl ether
 44 BP : 14.95 GWP : 1.07 MW : 146.00 TC : 12.20
 Rank: 24 38 76 57



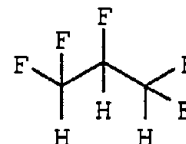
001493034 Methane, iododifluoro-
 45 BP : 21.60 exp GWP : 0.01 MW : 177.92 TC : 6.25
 Rank: 6 93 96 2



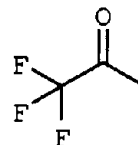
000686657 1,2-Difluorobutane
 46 BP : 8.56 GWP : 0.91 MW : 94.11 TC : 13.00
 Rank: 39 41 39 78



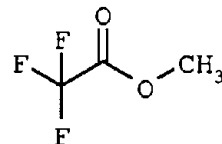
024270664 1,1,2,3,3-Pentafluoropropane
 47 BP : 39.30 exp GWP : 0.02 MW : 134.05 TC : 8.19
 Rank: 41 83 68 6



6112 1,1,1,3-Tetrafluoroacetone
 48 BP : 28.81 GWP : 0.01 MW : 130.00 TC : 11.00
 Rank: 13 90 60 36



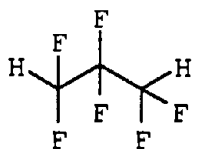
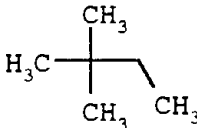
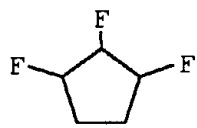
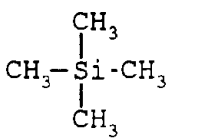
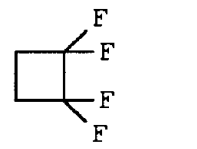
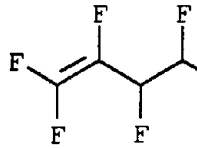
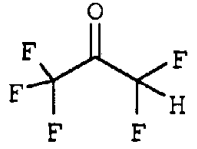
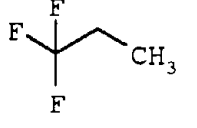
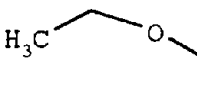
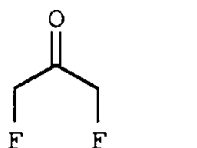
000431470 Methyl trifluoroacetate
 49 BP : 43.00 exp GWP : 0.05 MW : 128.00 TC : 10.90
 Rank: 49 71 57 26



BP = Boiling point in degrees C
 TC = Vapor thermal conductivity in mW/(m - K)
 MW = Molecular weight
 GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

exp = experimental value

Table 4. Final Ranking of Blowing Agent Candidates (continued)

000680002	1,1,2,2,3,3-Hexafluoropropane						
50	BP : 10.00 exp	GWP : 0.05	MW : 152.04	TC : 9.27			
	Rank: 35	75	82	12			
000075832	Butane, 2,2-dimethyl-						
51	BP : 50.00 exp	GWP : 2.32	MW : 86.18	TC : 13.20	exp		
	Rank: 69	26	28	81			
6108	1,2,3-Trifluorocyclopentane						
52	BP : 47.75	GWP : 1.25	MW : 124.00	TC : 12.00			
	Rank: 62	35	56	52			
000075763	Tetramethyl silane						
53	BP : 26.00 exp	GWP : 0.10	MW : 88.23	TC : 15.50			
	Rank: 8	63	33	102			
000374129	1,1,2,2-Tetrafluorocyclobutane						
54	BP : 0.76	GWP : 0.61	MW : 128.07	TC : 11.90			
	Rank: 59	44	59	45			
000680546	1,1,2,3,4,4-Hexafluoro-1-butene						
55	BP : -3.77	GWP : 7.07	MW : 164.00	TC : 11.00			
	Rank: 72	14	88	34			
000431710	2-Propanone, 1,1,1,3,3-pentafluoro						
56	BP : 15.28	GWP : 0.00	MW : 148.03	TC : 9.56			
	Rank: 22	96	77	15			
000421078	Propane, 1,1,1-trifluoro-						
57	BP : -13.00 exp	GWP : 0.25	MW : 98.07	TC : 11.00			
	Rank: 86	51	42	31			
000690222	Trifluoromethyl ethyl ether						
58	BP : 1.45	GWP : 1.07	MW : 114.00	TC : 12.50			
	Rank: 56	39	52	63			
000453145	1,3-Difluoroacetone						
59	BP : 49.87	GWP : 0.13	MW : 94.06	TC : 12.00			
	Rank: 67	60	37	48			

BP = Boiling point in degrees C

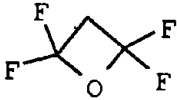
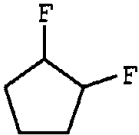
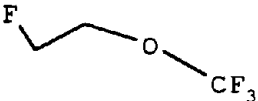
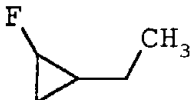
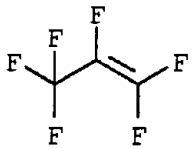
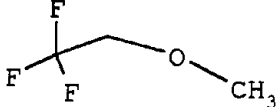
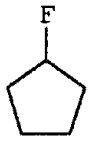
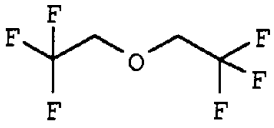
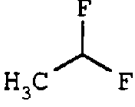
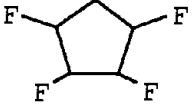
exp = experimental value

TC = Vapor thermal conductivity in mW/(m - K)

MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

Table 4. Final Ranking of Blowing Agent Candidates (continued)

154330402	1,1,3,3-Tetrafluorooxetane						
60	BP : 21.20 exp	GWP : 0.02	MW : 130.04	TC : 12.20			
	Rank: 10	82	63	58			
113742908	1,2-Difluorocyclopentane						
61	BP : 52.71	GWP : 2.31	MW : 106.00	TC : 12.50			
	Rank: 74	27	46	66			
000819498	1-Trifluoromethoxy-2-fluoroethane						
62	BP : 4.14	GWP : 0.73	MW : 132.00	TC : 12.10			
	Rank: 50	42	67	55			
050422769	1-Fluoro-2-ethylcyclopropane						
63	BP : 45.44	GWP : 1.31	MW : 88.00	TC : 14.50			
	Rank: 54	34	31	95			
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-						
64	BP : -28.00 exp	GWP : 7.04	MW : 150.02	TC : 10.47 exp			
	Rank: 97	15	81	22			
000460435	1-Methoxy-2,2,2-trifluoroethane						
65	BP : 1.45	GWP : 0.49	MW : 114.00	TC : 12.50			
	Rank: 55	48	51	62			
001481363	Fluorocyclopentane						
66	BP : 57.64	GWP : 3.46	MW : 88.00	TC : 13.30			
	Rank: 82	23	29	82			
000333368	Bis-2,2,2-trifluoroethyl ether						
67	BP : 9.50	GWP : 0.09	MW : 182.00	TC : 9.93			
	Rank: 38	64	99	17			
000075376	Ethane, 1,1-difluoro-						
68	BP : -25.00 exp	GWP : 0.03	MW : 66.05	TC : 11.50 exp			
	Rank: 94	76	8	40			
6109	1,2,3,4-Tetrafluorocyclopentane						
69	BP : 42.76	GWP : 0.53	MW : 142.00	TC : 12.00			
	Rank: 47	47	74	53			

BP = Boiling point in degrees C

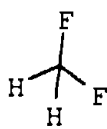
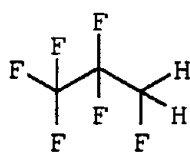
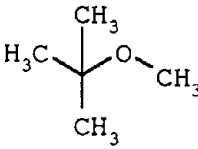
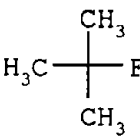
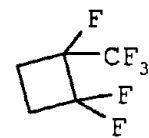
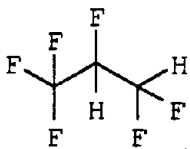
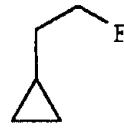
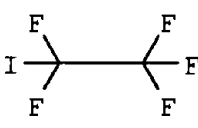
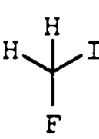
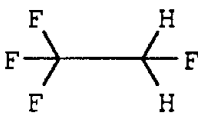
exp = experimental value

TC = Vapor thermal conductivity in mW/(m - K)

MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

Table 4. Final Ranking of Blowing Agent Candidates (continued)

000075105	Methane, difluoro-									
70	BP : -51.65 exp	GWP : 0.01	MW : 52.02	TC : 11.00	exp					
	Rank: 104	89	2	29						
000677565	1,1,1,2,2,3-Hexafluoropropane									
71	BP : -1.20 exp	GWP : 0.11	MW : 152.04	TC : 10.00						
	Rank: 63	62	83	18						
001634044	t-Butyl methyl ether									
72	BP : 55.00 exp	GWP : 2.82	MW : 88.00	TC : 14.40						
	Rank: 80	25	30	94						
000353617	Propane, 2-fluoro-2-methyl-									
73	BP : -5.02	GWP : 0.56	MW : 76.11	TC : 13.80						
	Rank: 73	46	23	91						
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane									
74	BP : 9.73	GWP : 0.61	MW : 178.00	TC : 12.10						
	Rank: 36	45	98	56						
000431630	1,1,1,2,3,3-Hexafluoropropane									
75	BP : 6.00 exp	GWP : 0.01	MW : 152.04	TC : 10.20	exp					
	Rank: 46	88	85	20						
069750681	2-Fluoroethylcyclopropane									
76	BP : 52.94	GWP : 1.14	MW : 88.00	TC : 14.50						
	Rank: 75	37	32	96						
000354643	Ethane, pentafluoroiodo-									
77	BP : 12.00 exp	GWP : 0.00	MW : 245.92	TC : 8.30						
	Rank: 32	100	103	7						
000373535	Methane, iodo fluoro-									
78	BP : 53.40 exp	GWP : 0.02	MW : 159.93	TC : 5.11						
	Rank: 77	79	87	1						
000811972	Ethane, 1,1,1,2-tetrafluoro-									
79	BP : -26.50 exp	GWP : 0.01	MW : 102.03	TC : 9.10	exp					
	Rank: 96	92	45	11						

BP = Boiling point in degrees C

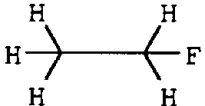
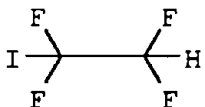
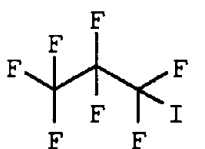
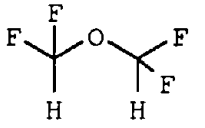
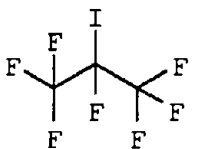
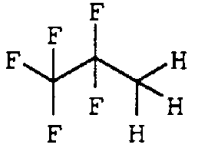
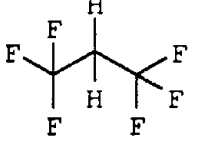
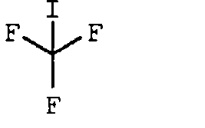
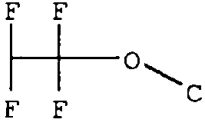
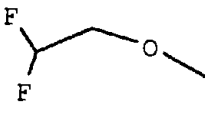
exp = experimental value

TC = Vapor thermal conductivity in mW/(m - K)

MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

Table 4. Final Ranking of Blowing Agent Candidates (continued)

000353366	Ethane, fluoro-									
80	BP : -37.70exp	GWP : 0.23	MW : 48.06	TC : 13.80	exp					
	Rank: 101	52	1	90						
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-									
81	BP : 41.00 exp	GWP : 0.00	MW : 227.93	TC : 7.45						
	Rank: 43	97	102	3						
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-									
82	BP : 40.00 exp	GWP : 0.00	MW : 295.93	TC : 8.06						
	Rank: 42	99	104	4						
001691174	Difluoromethyl ether									
83	BP : 4.70 exp	GWP : 0.02	MW : 118.03	TC : 12.50						
	Rank: 48	84	54	64						
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-									
84	BP : 38.00 exp	GWP : 0.00	MW : 295.93	TC : 8.54						
	Rank: 37	101	105	8						
001814886	1,1,1,2,2-Pentafluoropropane									
85	BP : -17.60exp	GWP : 0.19	MW : 134.05	TC : 11.50	exp					
	Rank: 88	55	72	41						
000690391	1,1,1,3,3,3-Hexafluoropropane									
86	BP : -0.07 exp	GWP : 0.00	MW : 152.04	TC : 10.10						
	Rank: 61	94	84	19						
002314978	Methane, trifluoroiodo-									
87	BP : -22.50exp	GWP : 0.12	MW : 195.91	TC : 8.06						
	Rank: 92	61	101	5						
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane									
88	BP : -12.54	GWP : 0.08	MW : 132.00	TC : 12.00						
	Rank: 84	65	64	47						
032778168	1-Difluoromethoxy-2,2-difluoroethane									
89	BP : -1.54	GWP : 0.02	MW : 132.00	TC : 12.00						
	Rank: 64	85	65	50						

BP = Boiling point in degrees C

exp = experimental value

TC = Vapor thermal conductivity in mW/(m · K)

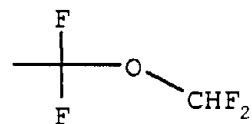
MW = Molecular weight

GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

Table 4. Final Ranking of Blowing Agent Candidates (continued)

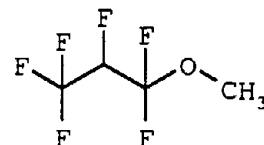
069948294 1-Difluoromethoxy-1,1-difluoroethane

90 BP: -12.54 GWP: 0.06 MW: 132.00 TC: 12.00
 Rank: 85 69 66 51



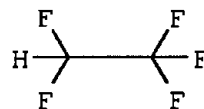
000382343 1,1,2,3,3-Pentafluoropropyl methyl ether

91 BP: -7.07 GWP: 0.08 MW: 182.00 TC: 11.00
 Rank: 78 66 100 30



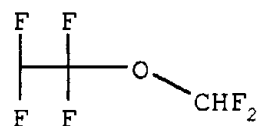
000354336 Ethane, pentafluoro-

92 BP: -48.50exp GWP: 0.00 MW: 120.02 TC: 10.90 exp
 Rank: 103 95 55 25



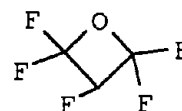
032778113 1-Difluoromethoxy-1,1,2,2-tetrafluoroethane

93 BP: -3.10 exp GWP: 0.05 MW: 168.00 TC: 11.50
 Rank: 71 74 93 42



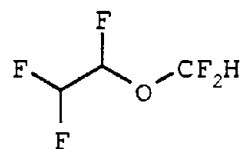
144109035 1,1,2,2,3-Pentafluorooxetane

94 BP: 3.40 exp GWP: 0.03 MW: 148.03 TC: 13.00
 Rank: 53 78 78 80



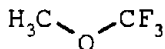
056281926 1-Difluoromethoxy-1,2,2-trifluoroethane

95 BP: -15.58 GWP: 0.02 MW: 150.00 TC: 11.70
 Rank: 87 80 80 44



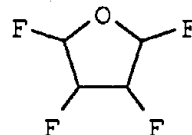
000421147 Trifluoromethyl methyl ether

96 BP: -24.10exp GWP: 0.07 MW: 100.04 TC: 13.70 exp
 Rank: 93 67 44 87



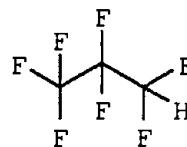
133360006 2,3,4,5-Tetrafluorotetrahydrofuran

97 BP: 49.77 GWP: 0.14 MW: 144.00 TC: 14.80
 Rank: 66 57 75 100



002252848 1,1,1,2,2,3,3-Heptafluoropropane

98 BP: -17.70exp GWP: 0.02 MW: 170.03 TC: 11.00
 Rank: 89 81 95 35

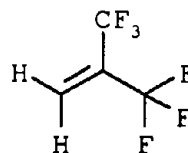


BP = Boiling point in degrees C
 TC = Vapor thermal conductivity in mW/(m - K)
 MW = Molecular weight
 GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec

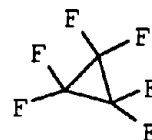
exp = experimental value

Table 4. Final Ranking of Blowing Agent Candidates (continued)

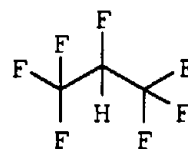
000382105 1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-
 99 BP: -29.10 GWP: 51.40 MW: 164.05 TC: 17.00
 Rank: 99 9 89 105



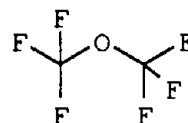
000931919 Hexafluorocyclopropane
 100 BP: -47.70 GWP: 0.00 MW: 150.00 TC: 10.90
 Rank: 102 102 79 28



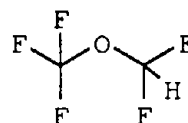
000431890 1,1,1,2,3,3,3-Heptafluoropropane
 101 BP: -18.70exp GWP: 0.00 MW: 170.03 TC: 11.00
 Rank: 91 98 94 33



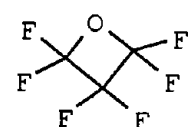
001479498 Trifluoromethyl ether
 102 BP: -58.70exp GWP: 0.00 MW: 154.01 TC: 12.70
 Rank: 105 103 86 72



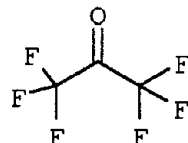
003822682 Trifluoromethyl difluoromethyl ether
 103 BP: -34.60exp GWP: 0.01 MW: 136.02 TC: 16.20 exp
 Rank: 100 91 73 104



000425821 1,1,2,2,3,3-Hexafluorooxetane
 104 BP: -28.20exp GWP: 0.00 MW: 166.02 TC: 13.70
 Rank: 98 104 90 88



000684162 2-Propanone, hexafluoro
 105 BP: -26.00exp GWP: 0.00 MW: 166.02 TC: 13.70 exp
 Rank: 95 105 91 89



BP = Boiling point in degrees C
 TC = Vapor thermal conductivity in mW/(m - K)
 MW = Molecular weight
 GWP = Atmospheric hydroxyl radical reaction rate in cu-cm/molecule-sec
 exp = experimental value

heading BP refers to ΔBP (in $^{\circ}C$), GWP refers to the hydroxyl radical rate constant (in $cm^3/molecule\text{-}sec \times 10^{12}$), MW refers to the molecular weight, and TC refers to vapor thermal conductivity in $mW/(m\ K)$.

This ranking exercise produced other interesting results which will be discussed in the following section. For example, unsaturated compounds in the ranking list may also undergo atmospheric reactions with ozone and/or nitrate radicals which would shorten their atmospheric lifetime and, thus, they should be moved to a higher rank in the GWP ranking criteria.

Perfluoroalkyl iodides do not react with hydroxyl radicals and, for this exercise, were ranked very low for GWP; however, this class of compounds is known to directly photodegrade in the atmosphere upon exposure to UV radiation. Therefore, the global warming potential would be considerably lower than indicated in the ranking exercise and these compounds should not be removed from further consideration based solely on this criteria.

A wide range of chemical compounds were considered for this project. Some of these compounds have not been previously discussed in the chemistry literature and, therefore, do not possess CAS Registry numbers. To facilitate the extensive electronic data manipulation operations utilized in this project, these compounds were provided with an artificial number, or a CAS Registry numbers for a closely related, generic species, or for one of two possible geometric isomers. These compounds are listed in Table 5.

Table 5. Compounds with Artificial CAS Registry Numbers

CAS No.	Name	Notes
129362-97-6	1,2,3,4-Tetrafluorocyclobutane	CAS Registry number is for generic compound, tetrafluorocyclobutane
6104	1,2,3-Trifluorocyclobutane	Compound does not exist in chemical literature
113742-90-8	1,2-Difluorocyclobutane	CAS Registry number is for the trans isomer
6108	1,2,3-Trifluorocyclopentane	Compound does not exist in chemical literature
6109	1,2,3,4-Tetrafluorocyclopentane	Compound does not exist in chemical literature
50422-76-9	1-Fluoro-2-ethylcyclopropane	CAS Registry number is for the trans isomer
6119	Trifluoromethoxy-methoxymethane	Compound does not exist in chemical literature

Task 3. Evaluation of Potential New Foam Blowing Agents

In order to efficiently evaluate potential new foam blowing agents, the compounds were placed in a series of fourteen groups based on chemical structure. The chemical structure of a compound ultimately determines the physical/chemical properties it will possess. By placing compounds in chemical groups, similarities can be discussed collectively and trends that represent differences can be identified. A complete listing of the chemicals compounds used in our scoring exercise sorted by chemical group is provided in Table 6. In addition to the overall rank, Table 6 also contains the order rank of each compound in each of the four criteria areas.

In the following, there are three areas of discussion on each group. A general section identifies the members of the groups along with a potentially wide-ranging discussion of areas that directly relate to their potential use as blowing agents. This may include a brief discussion

Table 6. Group Ranking of Blowing Agent Candidates

A. Cyclopentane and cyclopentene



1

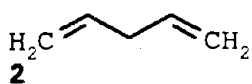
BP : 52 MW :9
GWP : 2 TC : 24



13

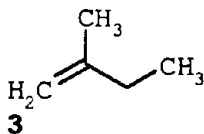
BP : 68 MW :11
GWP : 18 TC : 54

B. Simple olefins



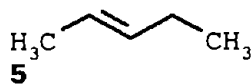
2

BP : 7 MW :10
GWP : 8 TC : 68



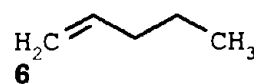
3

BP : 20 MW :13
GWP : 3 TC : 76



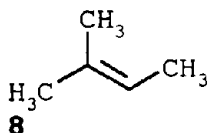
5

BP : 34 MW :12
GWP : 4 TC : 70



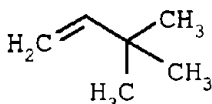
6

BP : 18 MW :14
GWP : 10 TC : 86



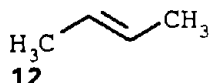
8

BP : 30 MW :15
GWP : 1 TC : 93



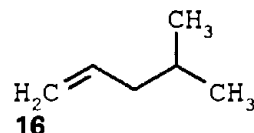
10

BP : 44 MW :26
GWP : 12 TC : 61



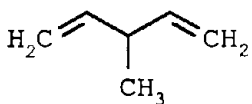
12

BP : 58 MW :3
GWP : 5 TC : 83



16

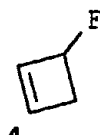
BP : 76 MW :25
GWP : 11 TC : 43



31

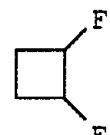
BP : 79 MW :24
GWP : 7 TC : 71

C. Cyclobutane analogues



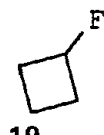
4

BP : 25 MW :17
GWP : 6 TC : 67



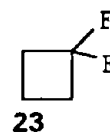
17

BP : 1 MW :34
GWP : 49 TC : 73



19

BP : 15 MW :20
GWP : 43 TC : 85



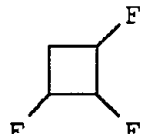
23

BP : 19 MW :35
GWP : 40 TC : 74



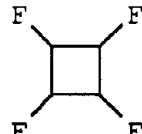
26

BP : 31 MW :5
GWP : 36 TC : 99



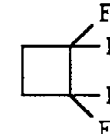
28

BP : 12 MW :48
GWP : 58 TC : 59



43

BP : 26 MW :58
GWP : 72 TC : 39

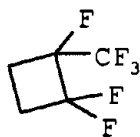


54

BP : 59 MW :59
GWP : 44 TC : 45

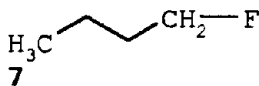
Table 6. Group Ranking of Blowing Agent Candidates (continued)

C. Cyclobutane analogues

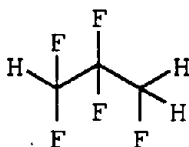


74 BP : 36 MW :98
GWP : 45 TC : 56

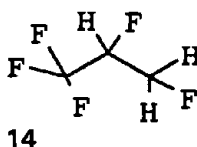
D. Fluorinated propanes and butanes



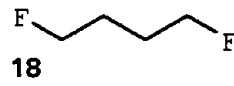
7 BP : 23 MW :22
GWP : 28 TC : 65



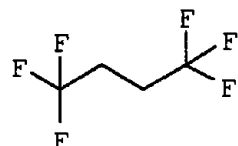
9 BP : 5 MW :69
GWP : 59 TC : 9



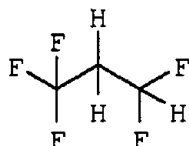
14 BP : 4 MW :70
GWP : 70 TC : 10



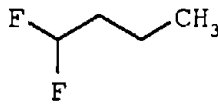
18 BP : 14 MW :38
GWP : 30 TC : 77



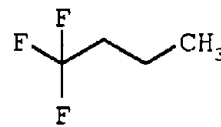
21 BP : 3 MW :92
GWP : 56 TC : 14



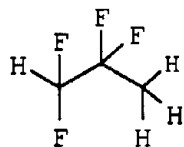
32 BP : 21 MW :71
GWP : 77 TC : 13



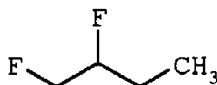
37 BP : 40 MW :40
GWP : 31 TC : 79



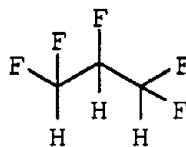
40 BP : 60 MW :49
GWP : 33 TC : 49



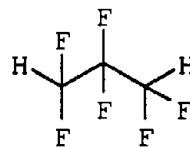
42 BP : 65 MW :53
GWP : 54 TC : 23



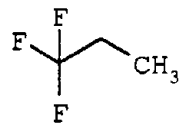
46 BP : 39 MW :39
GWP : 41 TC : 78



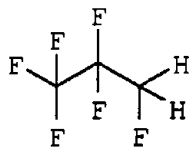
47 BP : 41 MW :68
GWP : 83 TC : 6



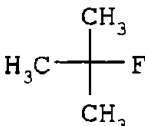
50 BP : 35 MW :82
GWP : 75 TC : 12



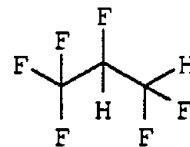
57 BP : 86 MW :42
GWP : 51 TC : 31



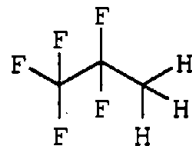
71 BP : 63 MW :83
GWP : 62 TC : 18



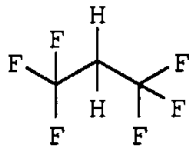
73 BP : 73 MW :23
GWP : 46 TC : 91



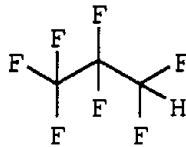
75 BP : 46 MW :85
GWP : 88 TC : 20



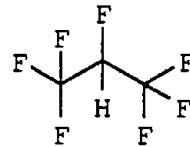
85 BP : 88 MW :72
GWP : 55 TC : 41



86 BP : 61 MW :84
GWP : 94 TC : 19



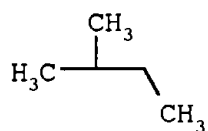
98 BP : 89 MW :95
GWP : 81 TC : 35



101 BP : 91 MW :94
GWP : 98 TC : 33

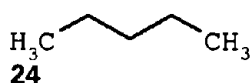
Table 6. Group Ranking of Blowing Agent Candidates (continued)

E. Pentanes and hexanes



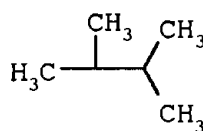
11

BP : 11 MW :18
GWP : 21 TC : 97



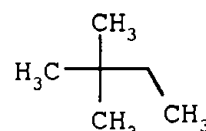
24

BP : 33 MW :19
GWP : 20 TC : 98



34

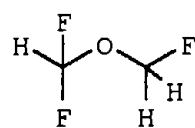
BP : 83 MW :27
GWP : 17 TC : 60



51

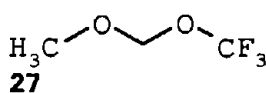
BP : 69 MW :28
GWP : 26 TC : 81

F. HFES



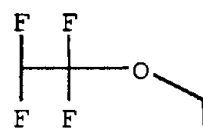
15

BP : 17 MW :43
GWP : 73 TC : 21



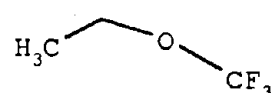
27

BP : 16 MW :61
GWP : 24 TC : 75



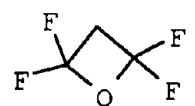
44

BP : 24 MW :76
GWP : 38 TC : 57



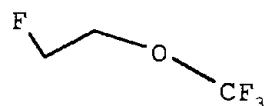
58

BP : 56 MW :52
GWP : 39 TC : 63



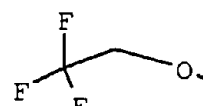
60

BP : 10 MW :63
GWP : 82 TC : 58



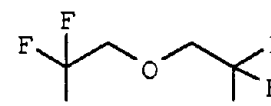
62

BP : 50 MW :67
GWP : 42 TC : 55



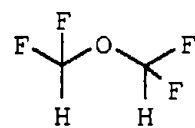
65

BP : 55 MW :51
GWP : 48 TC : 62



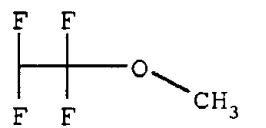
67

BP : 38 MW :99
GWP : 64 TC : 17



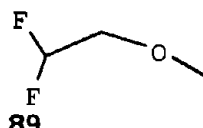
83

BP : 48 MW :54
GWP : 84 TC : 64



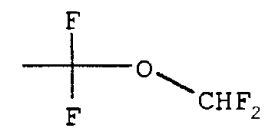
88

BP : 84 MW :64
GWP : 65 TC : 47



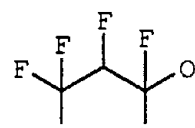
89

BP : 64 MW :65
GWP : 85 TC : 50



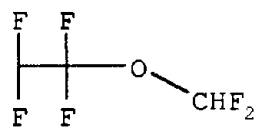
90

BP : 85 MW :66
GWP : 69 TC : 51



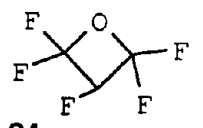
91

BP : 78 MW :100
GWP : 66 TC : 30



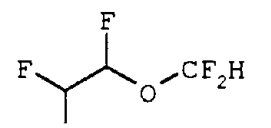
93

BP : 71 MW :93
GWP : 74 TC : 42



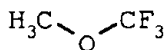
94

BP : 53 MW :78
GWP : 78 TC : 80



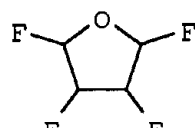
95

BP : 87 MW :80
GWP : 80 TC : 44



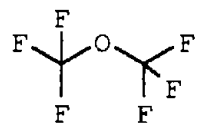
96

BP : 93 MW :44
GWP : 67 TC : 87



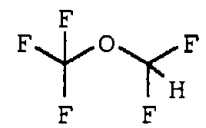
97

BP : 66 MW :75
GWP : 57 TC : 100



102

BP : 105 MW :86
GWP : 103 TC : 72

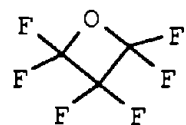


103

BP : 100 MW :73
GWP : 91 TC : 104

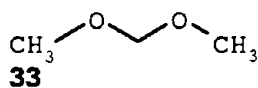
Table 6. Group Ranking of Blowing Agent Candidates (continued)

F. HFEs



104 BP : 98 MW :90
GWP : 104 TC : 88

G. Ethers



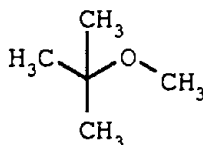
33

BP : 45 MW :21
GWP : 16 TC : 101



38

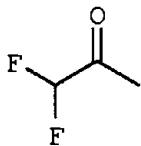
BP : 70 MW :6
GWP : 22 TC : 92



72

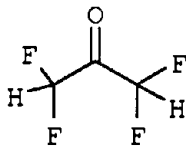
BP : 80 MW :30
GWP : 25 TC : 94

H. Carbonyl compounds



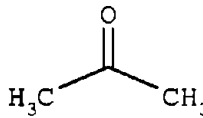
20

BP : 28 MW :36
GWP : 68 TC : 32



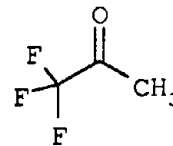
22

BP : 2 MW :62
GWP : 87 TC : 16



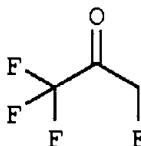
29

BP : 81 MW :7
GWP : 53 TC : 38



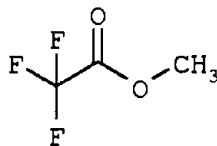
39

BP : 9 MW :50
GWP : 86 TC : 46



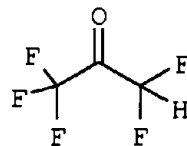
48

BP : 13 MW :60
GWP : 90 TC : 36



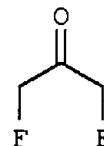
49

BP : 49 MW :57
GWP : 71 TC : 26



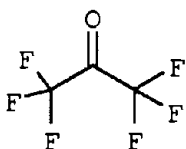
56

BP : 22 MW :77
GWP : 96 TC : 15



59

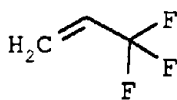
BP : 67 MW :37
GWP : 60 TC : 48



105

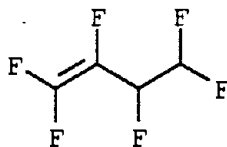
BP : 95 MW :91
GWP : 105 TC : 89

I. Fluorinated olefins



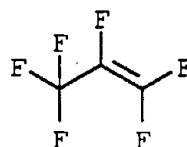
25

BP : 90 MW :41
GWP : 13 TC : 27



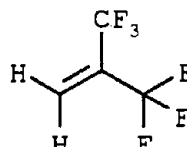
55

BP : 72 MW :88
GWP : 14 TC : 34



64

BP : 97 MW :81
GWP : 15 TC : 22

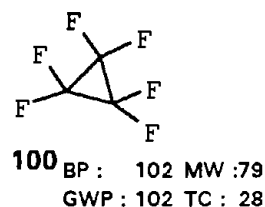
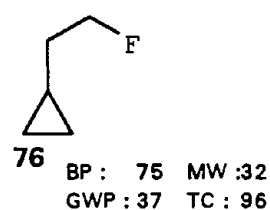
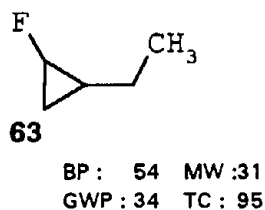
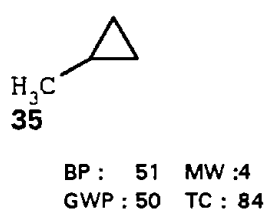
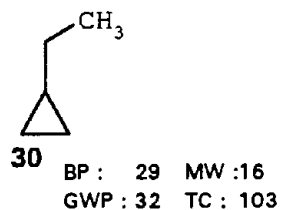


99

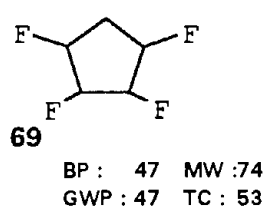
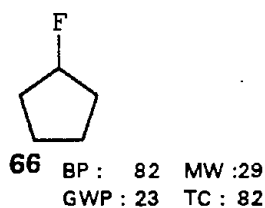
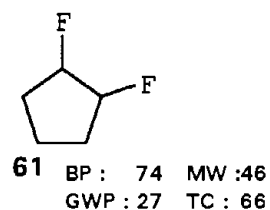
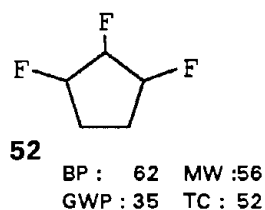
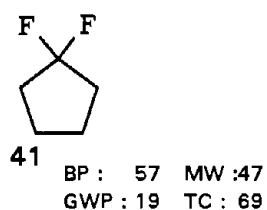
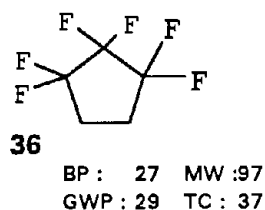
BP : 99 MW :89
GWP : 9 TC : 105

Table 6. Group Ranking of Blowing Agent Candidates (continued)

J. Cyclopropanes



K. Fluorinated cyclopentanes



L. Fluoroiodoalkanes

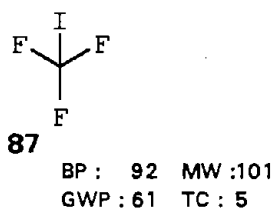
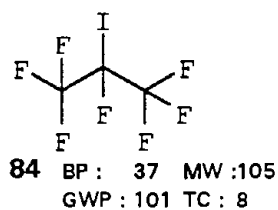
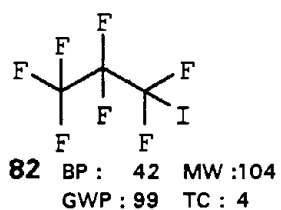
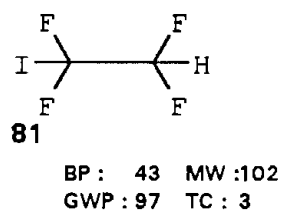
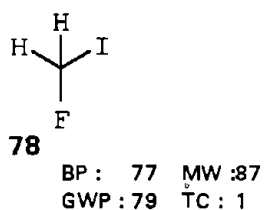
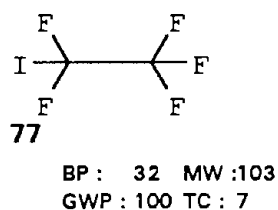
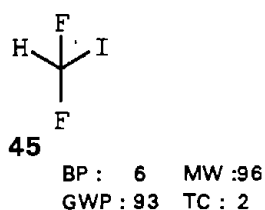
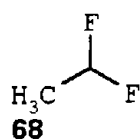
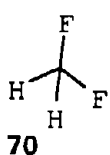


Table 6. Group Ranking of Blowing Agent Candidates (continued)

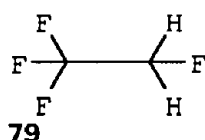
M. Fluorinated methane and ethanes



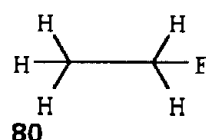
BP : 94 MW :8
GWP : 76 TC : 40



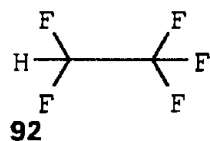
BP : 104 MW :2
GWP : 89 TC : 29



BP : 96 MW :45
GWP : 92 TC : 11

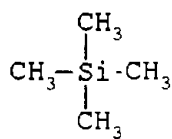


BP : 101 MW :1
GWP : 52 TC : 90



BP : 103 MW :55
GWP : 95 TC : 25

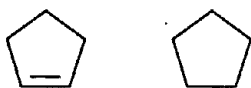
N. Silicon containing compounds



BP : 8 MW :33
GWP : 63 TC : 102

of physical/chemical properties. For a complete listing of physical/chemical properties, please refer to Appendices B, C, D, and E. The second section, manufacture, briefly indicates the commercial availability of the members of the group. The commercial availability of all compounds considered in the ranking exercise is provided in Appendix A. The determination of commercial availability was obtained by searching chemical company catalogues, articles from trade journals collected for this project, and on-line searches (using STN) of the CSCHEM database (for a limited number of compounds), as well as the chemical intuition of the authors of this report. Appendix A cannot be considered a comprehensive compilation of commercial availability, but rather an indication of the likelihood that a compound would need to be synthesized before experimental data could be obtained. The final section, toxicity, provides an indication of the potential health and ecological effects of the group members. Toxicity information was obtained by searching the Registry of Toxic Effects for Chemical Substances (RTECS) current awareness file, the Toxic Substances Control Act Test Submission (TSCATS) database (Santodonato, J. et al., 1987), and the Integrated Risk Information System (IRIS).

Group A - Cyclopentane and Cyclopentene



General

The commercialization of cyclopentane as a blowing agent for refrigerator and construction foams has been demonstrated by European manufacturers (Volkert, O., 1993; Walker, G. et al., 1993; Kuhn, E. and Schindler, P., 1993). The physical/chemical properties for cyclopentane, its cyclic geometry, and its commercialization as a blowing agent led to the investigation of closely related analogues. Cyclopentene was chosen for investigation as it would be expected to react more rapidly with photochemically produced hydroxyl radicals and, thus, would be expected to have a shorter atmospheric lifetime and corresponding lower GWP. Moreover, cyclic hydrocarbons tend to have lower vapor thermal conductivities than their straight-chain analogues and its physical/chemical properties would be expected to be similar to cyclopentane.

Using our ordering scheme, cyclopentene is the highest ranked alternative blowing agent for rigid polyurethane foams and cyclopentane ranked number 13. Given the commercial success of cyclopentane as a blowing agent, the relatively close ranking of cyclopentane and cyclopentene, and their comparable physical/chemical properties, these two compounds were combined into a single group.

The higher ranking of cyclopentene over cyclopentane is consistent with the overall premise of the ordering exercise. Cyclopentene has a slightly lower molecular weight than

cyclopentane, a lower vapor thermal conductivity, a boiling point closer to CFC 12, and a lower expected GWP. These differences in the four ordering criteria are all in a direction that would be expected to produce a better foam blowing agent.

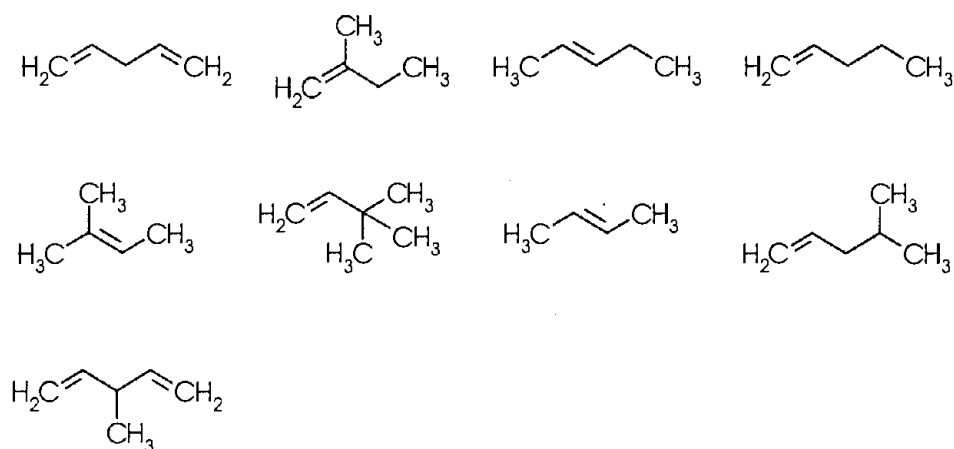
Manufacture

Both cyclopentene and cyclopentane are commercially available and relatively inexpensive. They are produced by the hydrogenation of cyclopentadiene which is obtained from the steam cracking of naphtha feedstocks (Griesbaum, K. et al., 1987; Griesbaum, K. et al., 1989).

Toxicity

Cyclopentene has an oral LD₅₀ in rats of 1656 mg/kg and a LD₅₀ in rabbits of 1231 mg/kg by dermal application as reported in RTECS.

Group B - Simple Olefins



General

The simple olefins group consists of hydrocarbons with four, five, or six carbons and at least one double bond. Similar to group A, the saturated pentane isomers of group E have been used commercially as blowing agents for rigid polyurethane foams (Ballhaus, H. and Hahan, H., 1993; Heilig, G. and Wiedermann, RE., 1993; Walker, G. et al., 1993; Kuhn, E. and Schindler, P., 1993). As a group, the unsaturated pentanes would be expected to have a lower vapor thermal conductivity than their saturated analogues as well as a shorter atmospheric lifetime. All else being equal, the compounds of group B ranked better than their saturated analogues in our ordering scheme.

There is a concern for the chemical reactivity of two members of this group, the dienes. This concern led to the removal of all conjugated dienes from our ranking lists. The two dienes in group B are not conjugated and, therefore, their reactivity may not be so high that they would be untenable as blowing agents. This higher expected reactivity, expressed in terms of the

expected atmospheric lifetime, is an important contributor to the high ranking of 1,4-pentadiene (ranked second overall). It is also important to note that this higher chemical reactivity of the dienes (and to some extent, all members of this group) is expected to be of consequence in the available purity of the blowing agent feedstock, stability in storage, and stability in the foam. No problems are expected to arise during the actual blowing of the foam.

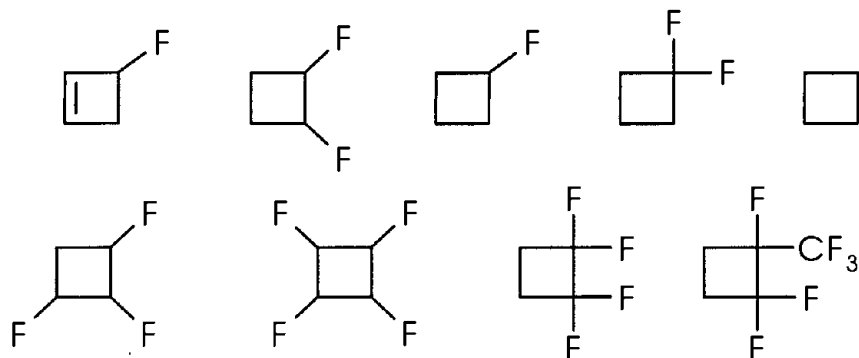
Manufacture

All members of this group are commercially available and are readily obtained from the thermal cracking of wet natural gas and petroleum fractions (Griesbaum, K. et al., 1989).

Toxicity

According to abstracted studies in TSCATS, concern for inhalation genotoxicity in mice for 2-methyl-2-butene and 2-methyl-1-butene exists. In RTECS, an LC_{50} of 425 ppm by inhalation in mice is reported for both compounds.

Group C - Cyclobutane Analogs



General

Group C is a novel group of compounds that have not previously been considered as foam blowing agents. Indeed, some members of this group have not been discussed in the chemical literature (that is, no CAS number has been assigned). The first member of this group, 3-fluorocyclobutene ranked as one of the top five candidates in the overall rank while the mono-, di-, trifluorocyclobutanes all ranked relatively closely to one another (17, 19, 23, and 28) as did the two tetrafluorocyclobutanes (43 and 54).

The reasons that members of this group ranked relatively well are due to their boiling point, relatively low molecular weight, and relatively rapid rate of atmospheric destruction. Their vapor thermal conductivity values are all pretty close together. Although not outstanding, their thermal conductivities are in the middle of the range [11-12 mW/(m K)] of chemicals considered during this project.

Cyclobutane itself was placed in this group because of its similar structural backbone. However, cyclobutane does not appear to offer any advantages over the use of cyclopentane as a blowing agent and is hampered by the expected higher cost relative to cyclopentane.

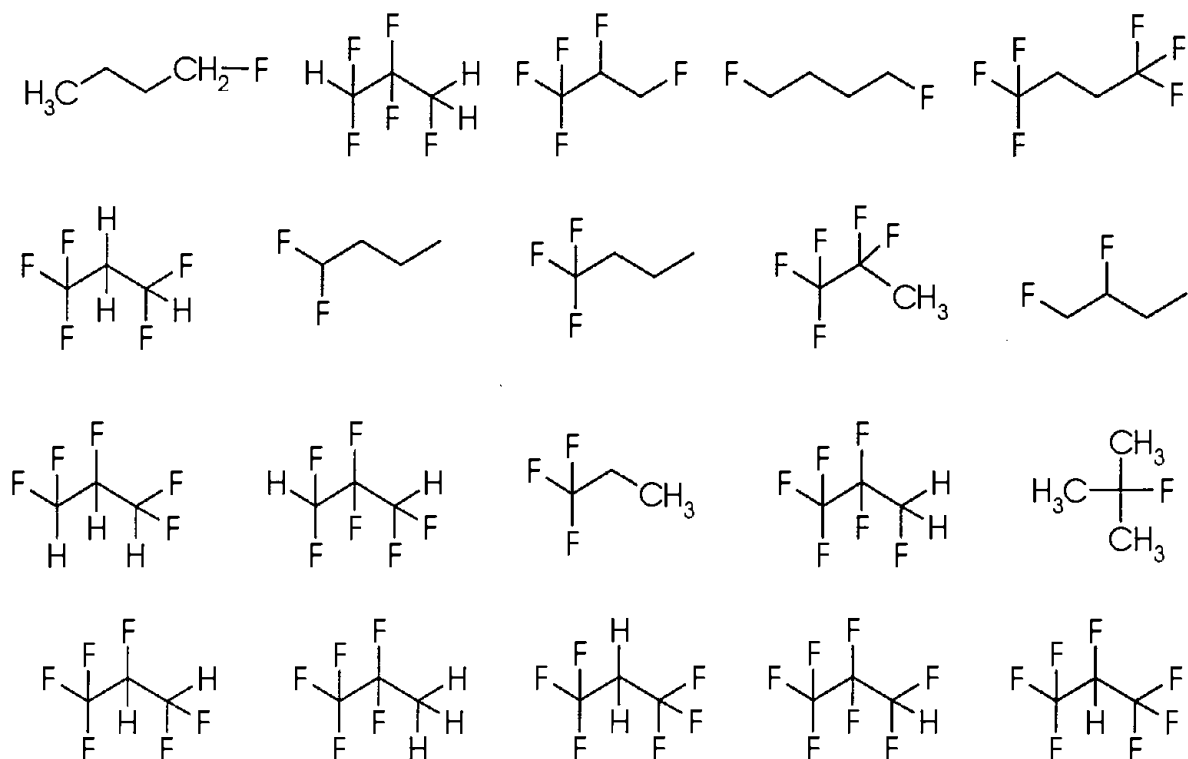
Manufacture

Cyclobutane is the only member of this group known to be commercially available. Of the fluorinated isomers, 1,1,2,2-tetrafluorocyclobutane used to be commercially available but it is not known if it is currently available. One of the interesting aspects of this group is that the mono-, di-, and trifluorocyclobutanes are ranked relatively close together. For this reason, it is not unreasonable to expect that a mixture of these compounds would also make a suitable blowing agent. This may offer some manufacturing benefits as a commercial synthesis of one isomer is likely to produce (or have as impurities) the others. If the final product was intended to be a mixture of the isomers, the synthetic process and the purification step would be simplified and the associated production costs would be lower.

Toxicity

No data were located.

Group D - Fluorinated Propanes and Butanes



General

This group is comprised of three and four carbon HFCs. Industrial concerns have expended significant effort looking at this group of compounds because they are expected to have similar physical/chemical properties to current blowing agents and refrigerants but do not contain chlorine like HCFCs. A complete discussion of HFC research is outside the scope of this document; however, industrial experiments often include foaming trials that provide an indication of the compound's usefulness as a blowing agent as well as the properties of the resulting foam. According to the literature, HFCs of this group with potential as blowing agent substitutes include HFC 356 (1,1,1,4,4,4-hexafluorobutane) and 227 (1,1,1,2,3,3,3-

heptafluoropropane) (Ball, EE. and Lamberts, WM., 1993; Yu-Halada, LC. and Reichel, CJ., 1993).

An interesting result from the ranking exercise on this group of compounds was that both the number and the position of the fluorine substituents strongly affected the overall score. For example, 1-fluorobutane ranked 7 and 1,1,1,2,3,3,3-heptafluoropropane ranked 101; there was not a linear correlation based on the number and position of fluorine atoms between these two extremes.

There is some evidence that some of the HFCs, particularly those with a CF_3 group, may not be as environmentally benign as originally believed. Although these experiments were performed on fluorinated ethanes (Ravishankara, AR. et al., 1994; Wallington, TJ. and Schneider, WF., 1994), the authors found that trifluoromethoxy radicals could be formed which could participate in the catalyzed destruction of stratospheric ozone. The authors have stated that their kinetic models indicate that the ozone depletion potential from these compounds is expected to be negligible.

In the atmosphere, HFCs containing a CF_3 group may also react with photochemically produced hydroxyl radicals producing trifluoroacetate. Trifluoroacetate can then undergo atmospheric removal, most likely by a wet deposition process. It has recently been shown (Visscher, PT. et al., 1994) that trifluoroacetate can biodegrade to fluoroform (trifluoromethane). Fluoroform is a volatile compound with a relatively long atmospheric half-life. Fluoroform may also be a potential ozone-depleting compound (Chemical Marketing Reporter, 1994) as recent workers have suggested that molecules containing the CF_3 group may represent a special case of fluorine-catalyzed ozone loss through cycles involving trifluorooxy and peroxy radicals (Ravishankara, AR. et al., 1994) although others have indicated that these reactions are not viable (Wallington, TJ. et al., 1994). Given that research in this area has just begun, the best HFC

blowing agent replacements from this group (as well as group M) may be those that do not contain a CF_3 group.

A number of workers have determined that highly fluorinated HFCs are expected to have long atmospheric lifetimes (Ravishankara, AR. et al., 1993; Zhang, Z. et al., 1994) , as determined by slow experimental rates constants for the gas-phase reaction with hydroxyl radicals. These result are consistent with the method for ranking GWP used in this project as the highly fluorinated HFCs ranked relatively low in the GWP ranking criteria.

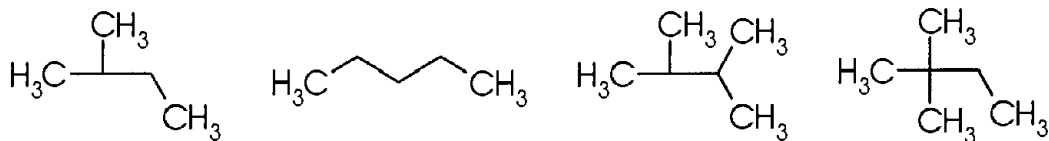
Manufacture

Some members of this group are available commercially or have been synthesized from research purposes. To our knowledge, none of the HFCs from this group are in large scale commercial production (like those of group M, fluorinated ethanes and methane). Appendix A has more information on the availability of these group members.

Toxicity

1,4-difluoro-butane has a LD_{50} in mice of 3400 $\mu\text{g/kg}$ by intraperitoneal injection and 1,1,1,3,3,3-hexafluoropropane has a LC_{50} in mice of 44 pph/10 minutes by inhalation as reported in RTECS.

Group E - Pentanes and Hexanes



General

The five and six carbon alkanes that met the boiling point criteria were placed in this group. They ranked relatively close together in the ordering exercise at positions 11, 24, 34, and 51. Pentane and *iso*-pentane have been used commercially as blowing agents for rigid polyurethane foams (Taverna, M. and Corradi, P., 1994; ES&T, 1994).

Manufacture

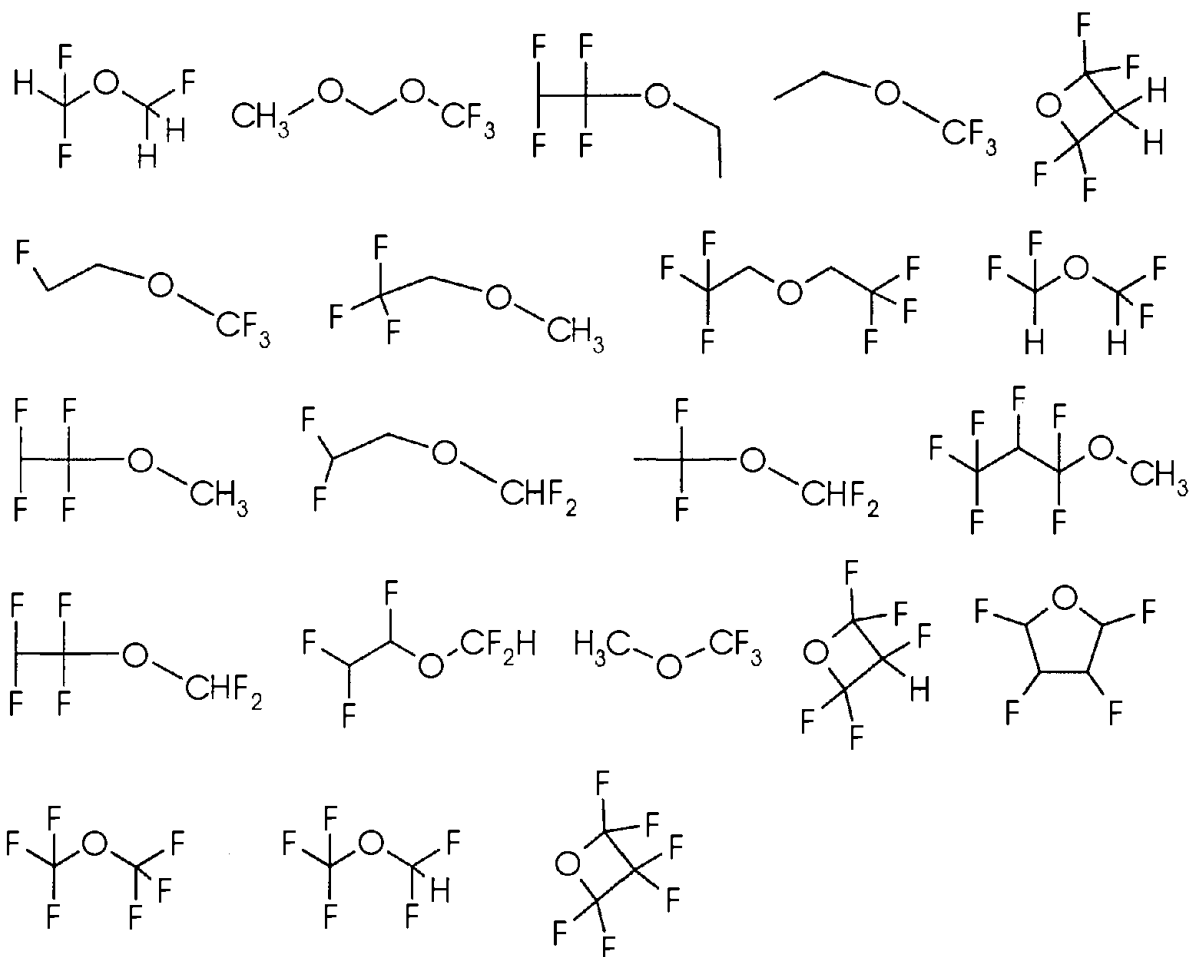
The members of this group are all commercially available and are fairly inexpensive. n-Pentane is obtained directly from the distillation of petroleum fractions and *iso*-pentane is obtained from the acid catalyzed isomerization of *n*-pentane (Griesbaum, K. et al., 1989). The other members of this group are obtained by the cracking of petrochemical feedstocks followed by distillation.

Toxicity

According to abstracted studies in TSCATS, toxicity following subchronic exposure was observed in male rats receiving 0.5 or 2.0 g/kg n-pentane once daily by oral gavage. For *iso*-pentane and 2,3-dimethyl butane, there is some data that indicates a concern for oral subchronic

toxicity in rats. In RTECS an LC_{50} in rats of $364 \text{ g/m}^3/4 \text{ hrs}$ by inhalation and a intravenous LD_{50} in mice of 446 mg/kg are reported for pentane.

Group F - HFEs



General

The members of this group consist of both the cyclic and acyclic fluorinated ethers. Because this group encompasses such a large variety of fluorination patterns and ether side chains that represent large differences in all four of the ranking criteria, no generalized trends can be made concerning this group. Some members possess all the requisite properties to be considered highly desirable as blowing agents.

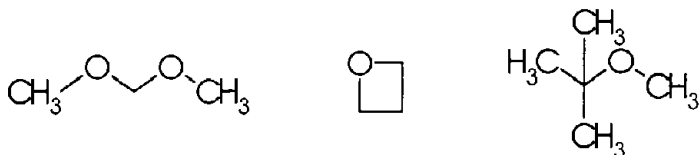
Manufacture

Only one member of this group is available commercially, bis-2,2,2-trifluoroethyl ether, and a number have been synthesized in small quantities for research purposes.

Toxicity

Bis-2,2,2-trifluoroethylether has a LD₅₀ in rats of 1260 mg/kg by intraperitoneal injection and a LD₅₀ in mice of 46 mg/kg by intravenous injection.

Group G - Ethers



General

The ethers from the initial list of compounds that met the boiling point criteria for this project were grouped together. Although these compounds ranked relatively well in GWP and molecular weight and reasonably well in boiling point, their thermal conductivities were among the highest of the compounds that were looked at.

Manufacture

All compounds in this group are commercially available. Methyl-*tert*-butyl ether is produced in billions of pounds annually by the catalyzed reaction of methanol with *iso*-butene (Kiem, W. and Roper, M., 1985). Dimethoxy methane is produced by the reaction of formaldehyde and methanol (Falbe, J. et al., 1985).

Toxicity

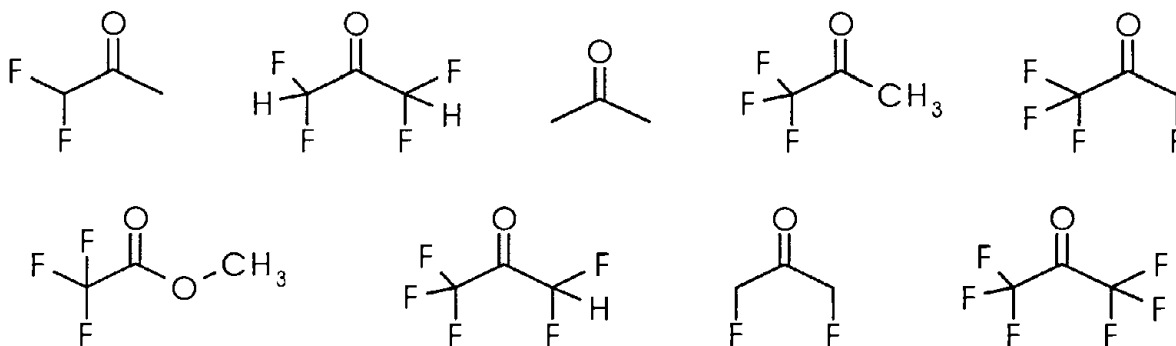
According to abstracted studies in TSCATS, chronic exposure to relatively high levels of methyl-*tert*-butyl ether (4,000-8,000 ppm) caused progressive nephrosis or nephropathy in the kidneys in male rats; exposure of male and female rats for long periods during mating and gestation resulted in some developmental affects. High concentrations also had a sedative affects.

Methyl-*tert*-butyl ether has an oral LD₅₀ in rats of 4 g/kg, a LC₅₀ in rats of 23576 ppm/4 hrs by inhalation, a LD₅₀ in rats of >148 mg/kg by intraperitoneal injection, and a LC₅₀ in mice 141 g/m³/15 minutes by inhalation as listed in RTECS.

Methyl-*tert*-butyl ether has an oral LD₅₀ in rats of 3899 mg/kg with ataxia and central nervous system depression noted at 1900 to 3160 mg/kg, and the 4-hour inhalation LC₅₀ in rats was 39,000 ppm resulting in irritation and prostration (Bosch, SJ. and Basu, DK., 1992). In repeat exposure oral studies in rats, 14, and 90 days, the lowest effective dose was 100 mg/kg/day which produced diarrhea, while doses greater than 300 mg/kg/day produced changes in organ weight. In repeat exposure inhalation studies in rats and mice (9 and 13 exposures; 6 hours/day), exposure produced irritation of the respiratory tract at 2970 ppm and ataxia at 4000 ppm. Methyl-*tert*-butyl ether had little effect on reproduction in a one and two generation inhalation study except at exposure levels in the range of 1200 to 3300 ppm in rats, mice, and rabbits.

According to abstracted TSCATS studies, dimethoxymethane has a LD₅₀ for rats of 7.46 ml/kg of body weight by oral gavage and 16.0 ml/kg of body weight for rabbits by dermal application and the LT₅₀ for saturated vapor inhalation was 19.8 for male rats and 25.5 minutes for females. Single applications of 5 g/kg dimethoxymethane resulted in no deaths with rabbits. Dimethoxymethane has a LC₅₀ in rats of 15,000 ppm by inhalation, a LC₅₀ in mice of 57 g/m³/7 hrs by inhalation, and a LD₅₀ in rabbits of 5,708 mg/kg orally as listed in RTECS.

Group H - Carbonyl Compounds



General

This group is composed mainly of fluorinated acetone isomers including acetone itself, and a fluorinated ester. Although these compounds ranked well in the scoring exercise, there is a concern, especially for the highly fluorinated compounds, that they may react with the isocyanate groups in the foam feedstocks. This is due to the high electronegativity of the fluorine groups withdrawing electron density from the carbonyl compound such that a stable ketal could be formed. For this reason, it is suggested that they be tested in foaming trials before they are recommended as HCFC alternatives. Acetone itself has been utilized successfully in foaming trials (Kaufman, CM. and Overcash, MR., 1993).

Manufacture

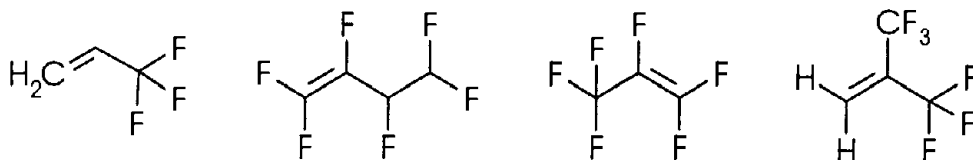
Acetone is an import industrial chemical and is widely available. Some of the fluorinated compounds are available in research quantities from commercial sources such as Aldrich Chemical Company. In general, the synthesis of the remaining members of this group is not

expected to be overly troublesome due to the ease of placing substituents next to a carbonyl group.

Toxicity

According to abstracted studies in TSCATS, there is a concern for developmental and reproductive toxicity in rats for hexafluoroacetone. Hexafluoroacetone causes testicular damage, bone marrow effects, and kidney damage in rats, and increases lung weight in dogs (Kennedy, GL., 1990). Acetone has an oral LD₅₀ in rats of 5800 mg/kg, a LC₅₀ in rats of 50100 mg/m³/8 hrs by inhalation, LD₅₀ in rats of 5500 mg/kg by intravenous injection, an oral LD₅₀ in mice of 3 g/kg, a LD₅₀ in mice of 1297 mg/kg by intraperitoneal injection, an oral LD₅₀ in rabbits of 5340 mg/kg, a LD₅₀ in rabbits of 20 g/kg by dermal application, and a LD₅₀ in guinea pigs of >9400 mg/kg by dermal application as reported in RTECS. 1,1,1,3,3,3-Hexafluoro-2-propanone has an oral LD₅₀ in rats of 191 mg/kg and a LC₅₀ in rats of 275 ppm/3 hrs by inhalation. All fluorinated members of this group that are sold by Aldrich are listed as lachrymators which would require exposure controls to reduce occupational exposure.

Group I - Fluorinated Olefins



General

The fluorinated olefins were investigated as they were expected to have a number of properties that offered advantages over their saturated analogues, the HFCs. These properties were a lower expected vapor thermal conductivity and shorter atmospheric lifetime and, of course, a somewhat lower molecular weight. Although the members of this group did rank relatively high in the GWP scoring, modest gains in molecular weight were more than offset by unexpected large drops in boiling point. Identifying new members of this group that better balance molecular weight (i.e., not too high due to a high degree of fluorination) and boiling point (i.e., one that is not a gas at room temperature) may produce a highly ranking blowing agent substitute.

Manufacture

Two members of this group are commercially available, 3,3,3-trifluoro-1-propene and 1,1,2,3,3,3-hexafluoro-1-propene; the former is a relatively high volume feedstock for polypropylene plastics.

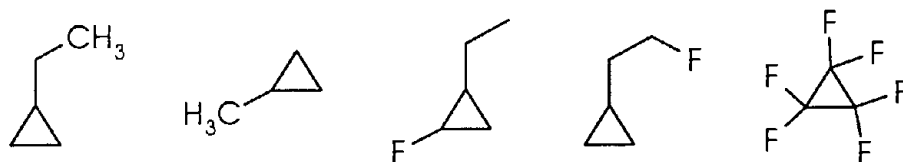
Toxicity

According to abstracted studies in TSCATS, the approximate lethal inhalation concentration of hexafluoropropene in rats was 735 ppm. Hexafluoropropene was classified as weakly positive for clastogenicity in male mice. For hexafluoro-*iso*-butylene, there is a concern for mutagenicity in mice and bacteria. For 3,3,3-trifluoropropene, there is a concern for acute toxicity by inhalation in mice with an LC₅₀ value of 1.75 g/L (445,000 ppm). It was also classified as mutagenic in the Ames assay.

Hexafluoro-propene has a LC₅₀ in rats of 1200 mg/m³/4 hrs by inhalation and a LC₅₀ in mice of 750 ppm/4 hrs by inhalation as reported by RTECS. 3,3,3-Trifluoro-2-(trifluoromethyl)-propene has a LC₅₀ in rats of 1425 ppm/4 hrs by inhalation and 3,3,3-trifluoropropene has a LC₅₀ in mice of 1691 g/m³/2 hrs by inhalation.

The fluorinated olefin perfluoro-*iso*-butene appeared on the initial list of potential blowing agent substitutes. This compound is listed in the Chemical Weapons Convention treaty (C&E News, 1993) because it is extremely toxic (Kennedy, GL., 1990) and, therefore, it was removed from further consideration. The toxicity of perfluoro-*iso*-butene arises from the formation of hydrofluoric acid by hydrolysis (in the lung tissue). The geometric isomer perfluoro-2-butene does not display this high level of toxicity. Because of these large changes in toxicity with relatively minor structural changes, more thorough toxicological investigation of the members of this group is required before they can be considered acceptable blowing agent substitutes.

Group J - Cyclopropanes



General

Little experimental data are available for this novel group of alternative blowing agents. Surprisingly, the non-fluorinated compounds in this group ranked higher than the fluorinated one. This may be an artifact of the boiling point term in the scoring exercise as the regression equations used in the estimation of boiling points may not work well for the cyclopropane functional group. An interesting area for future work would be to obtain experimental data for this group of compounds.

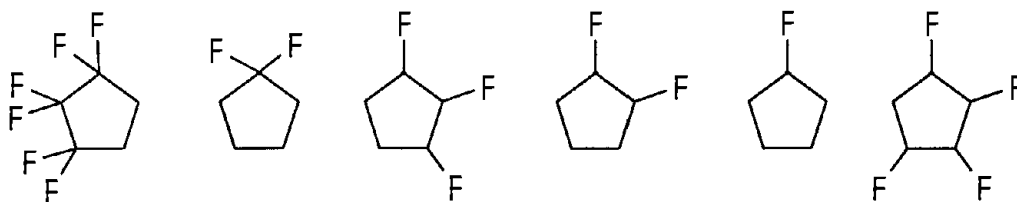
Manufacture

None of the compounds in this group are commercially available.

Toxicity

No data were located.

Group K - Fluorinated Cyclopentanes



General

With the commercial success of cyclopentane as a blowing agent as well as its high ranking in this scoring exercise, fluorinated cyclopentanes were considered for investigation in this study. To the best of our knowledge, members of this group have not previously been considered as blowing agents. The interest in these compounds was based on an expected decrease in the vapor thermal conductivity with the addition of fluorine groups. Similar to the fluorinated cyclobutanes, the members of this group ranked relatively close together (position 36 to 69) but, surprisingly, lower than cyclopentane itself. Given the potential for relatively large errors in estimated physical/chemical properties for cyclic compounds (as discussed above for the cyclobutane group) experimental measurements would aid in the assessment of the potential of these compounds as alternative blowing agents.

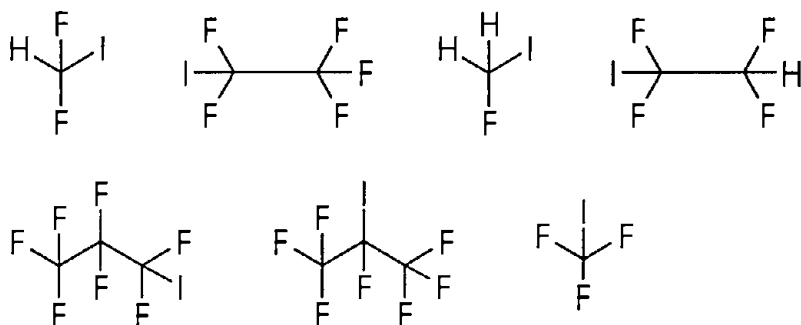
Manufacture

No members of this group are commercially available.

Toxicity

No data were located.

Group L - Fluoroiodoalkanes



General

Consideration of fluoriodoalkanes arose from their initial marketing as a halon and CFC replacement by a small research organization (Nimitz, J. and Lankford, PE., 1993; Lankford, PE. and Nimitz, J., 1993). The potential advantages from this class of compounds come from their expected low vapor thermal conductivity (due to their high degree of fluorination) and expected low atmospheric lifetime due to direct photolysis of the carbon-iodine bond. A major disadvantage of the members of this group is their high molecular weight.

Members of this group possessed the lowest overall vapor thermal conductivity; the seven members ranked 7th, 1st, 8th, 4th, 2nd, 5th, and 3rd in order of their appearance as shown above. In the molecular weight category, all members of this group ranked near the bottom, as expected.

Overall, the fully fluorinated members of this group did not score very well. The best showing was for pentafluoroiodoethane at position 77. It is important to note that the fully fluorinated members of this group could not be ranked for GWP using our scoring criteria. We based the GWP on the atmospheric half-life, which, in turn, was determined from the atmospheric reaction rate with photochemically produced hydroxyl radicals. For a saturated

compound to react with hydroxyl radicals in the atmosphere, it must contain a hydrogen atom (at least within the restraints of our estimation program). Therefore, the fully fluorinated members of this group scored at the very bottom in the GWP category. Moreover, the three members of this group that contain a hydrogen atom were also estimated to be essentially unreactive towards atmospheric hydroxyl radicals and, thus, also scored near the bottom of the GWP category.

This group of compounds is unique in that of all the different types of compounds looked at for this project, the fluoriodoalkanes are the only ones that are expected to undergo efficient atmospheric removal by a process other than oxidation by hydroxyl radicals. A carbon-iodine bond is well known to be susceptible to photolysis. The estimated atmospheric lifetime of methyl iodide is 5 days (Rasmussen, RA. et al., 1982; Chameides, WL. and Davis, DD., 1980). Although experimental evidence is lacking, the members of this group are expected to have short atmospheric lifetimes as the fluorine substituents should not significantly diminish the rate of carbon-iodine photolysis. Therefore, the members of this group are not expected to have a high GWP, at least not as high as our ordering exercise suggests.

The largest potential drawback of the members of this group is, therefore, their high molecular weight. The low vapor thermal conductivity and other desirable properties of some members of this group dictate that they should be given further consideration as potential polyurethane blowing agent substitutes, although their high molecular weights are likely to increase the cost associated with the production of the rigid foam.

Manufacture

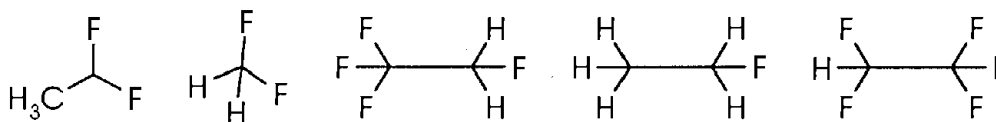
Iodofluoromethane, iododifluoromethane, and 1-iodo-1,1,2,2-tetrafluoroethane are the members of this group that are not commercially available. Trifluoriodomethane is undergoing

extensive research as a replacement for the fire-fighting agent Halon 1301 and ASTM is currently developing a research and testing material specification for this compound (ASTM, 1994). The other members of this group are available in research quantities (Nimitz, J. and Lankford, PE., 1993).

Toxicity

Heptafluoro-1-iodo-propane has a LC_{50} in mice of $404 \text{ g/m}^3/2 \text{ hrs}$ by inhalation as reported in RTECS.

Group M - Fluorinated Methane and Ethanes



General

This is the second group of HFCs and is limited to methane and ethane analogues. The general properties for this group are the same as those discussed for Group D. In general, this group did not score very well in our ordering exercise due, mainly, to their low boiling points (all members of this group are a gas at room temperature). Some members of this group that show promise in the literature as blowing agent replacements include HFC 143 (1,1,2-trifluoroethane) and 134a (1,1,1,2-tetrafluoroethane) (Barthelemy, PP. et al., 1993; Cecchini, C. et al., 1993; Yu-Halada, LC. and Reichel, CJ., 1993) .

Manufacture

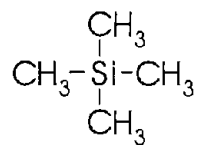
Several commercial plants have recently come on line to provide large amounts of HFC 134a (1,1,2,2-tetrafluoroethane), 125 (pentafluoroethane), and 143a (1,1,1-trifluoroethane) to be used as R502 and CFC 12 replacements in refrigeration units.

Toxicity

According to an abstracted study in TSCATS, 1,1-difluoroethane has an oral LD₅₀ greater than 1500 mg/kg in rats although there is some evidence for sub-chronic inhalation toxicity at

very high concentration levels. For 1,1,2,2-tetrafluoroethane, there is a concern for a teratologic effects by inhalation in rats.

Group N - Silicon Containing Compounds



General

In the course of this project, the investigation of silicon compounds was considered, given the well known chemical inertness and utility of many silicon containing materials. For many of the compounds under consideration, however, experimental boiling points and thermal conductivity values were not available. Indeed, Task 1 of this project involved the determination of a method for estimating vapor thermal conductivity values for silicon containing compounds.

Only one of the approximately twenty silicon compounds considered in this project possessed a boiling point appropriate for the final scoring exercise, tetramethylsilane. Although tetramethylsilane ranked 53rd overall, it came near the very bottom in the vapor thermal conductivity ranking.

Manufacture

Tetramethylsilane is widely available.

Toxicity

No data were located.

Information Gaps

The research described herein represents a systematic search to screen a large number of compounds to identify chemical candidates as substitutes for CFCs and HCFCs used for making polyurethane foam insulation products. A wide variety of chemical compounds were considered for this project. Some of these compounds were initially proposed as alternative blowing agents by commercial, governmental, or private research organizations and some were first considered as a blowing agent substitute in this project. When screening a large number of chemical compounds for any research project, initial effort is best spent focusing on the collection of readily available information. This project has collected, compiled, reviewed, and analyzed extensive amounts of readily available information and has identified, defined, and prioritized those compounds and chemical groups that hold the highest potential to become viable third-generation blowing agents based on this information. Additional information is needed before a select list of the best blowing agent replacements can be obtained. Several areas of research that would aid in this endeavor are described below.

Additional experimental information to fill existing data gaps on the boiling point and thermal conductivity would help evaluate new blowing agents. This effort would involve searching the chemical literature to identify papers where the compound of interest is specifically discussed, a process that is overly resource intensive to perform during a screening study. This would also allow experimental sources of other physical/chemical properties such as specific gravity, heat of vaporization, and flammability limits to be identified, compiled, and considered. Also, as noted in our report, the boiling points that were used for the vapor thermal conductivity estimates were prepared using a less precise method. It would be a worthwhile exercise to re-estimate the vapor thermal conductivities using the more accurate boiling point estimates.

It may be desirable to add other ranking criteria for sorting the alternative blowing agent candidates. Also, adding weights to the ordering criteria will better differentiate the blowing agent candidates. For example, molecular weight is probably not linear in importance in identifying third generation blowing agents relative to boiling point and GWP.

Another area that needs further examination is the flammability of potential alternatives. The CFCs and HCFCs exhibit low flammability characteristics. However, the commercial use of cyclopentane (Volkert, O., 1993; Walker, GW. et al., 1993; Kuhn, E. and Schindler, P., 1993) demonstrates that highly flammable materials can be used, but require additional, often expensive safety precautions. Information on flammability should be collected and estimates calculated for chemicals lacking experimental data.

Other information that would aid in the development of blowing agent candidates would be the commercial availability and ease of synthesis of the blowing agent candidates. Although all readily available blowing agent candidates were identified for this project, many of the compounds may be available from speciality chemical or overseas manufacturers. If a commercial source for a blowing agent candidate cannot be identified, the compound-specific literature search described above would also provide details of successful laboratory-scale synthesis routes that could be utilized to produce sufficient quantities of the compound for foaming trials and physical/chemical property measurements.

Information that would be useful in establishing the likelihood of a blowing agent candidate holding potential to attain commercial viability is detailed toxicological data. Because of resource limitations, only screening searches of the available literature were possible. A more in-depth review would have two stages. The first would be a complete compound-specific literature search of the toxicology literature followed by the review and analysis of all

experimental data retrieved. Data would be reviewed in the areas of acute, subchronic, chronic, neurological, reproductive, developmental, carcinogenic, and immunological effects. For those compounds that do not possess experimental toxicology data as well as for those that possess data gaps, the second stage would be to develop simple structure/activity relationships based on functional moieties to predict the importance of the above adverse affects.

Additional information on the use of mixed solvent systems as blowing agents could be valuable. The unique capability of UNIFAC activity coefficients to represent vapor-liquid and liquid-liquid equilibria for binary and multi component mixtures containing a wide variety of compounds such as hydrocarbons, ketones, esters, nitriles, and so on (Reid, RC., et al., 1987) could be used in this identification. Investigation of mixed solvent systems as blowing agents is advantageous because it will allow a blowing agent to be designed by blending the properties of one or more chemical substances. For example, fluoriodomethane ranked number 1 in the vapor thermal conductivity, but ranked poorly in boiling point criteria. By mixing this compound with, for example, 1,2-difluorocyclobutane which ranked number 1 in the boiling point criteria, a new blowing agent system that offers advantages over each of the individual components can be studied. Moreover, the UNIFAC method allow the proportions of each component of the mixture to be varied until the desired characteristics can be maximized.

UNIFAC is particularly appropriate for these calculations since it is the only general method for determining the properties of chemical mixtures at different temperatures. This method will allow desired physical/chemical properties to be reached by blending two or more compounds rather than by designing, synthesizing, and testing a large number of chemical compounds. A number of blowing agent candidates from Table 4 would be selected based on their unique physical/chemical properties. These compounds would then be blended using the

UNIFAC approach to achieve the optimum range of values for thermal conductivity, solubility, and flammability as well as other important properties. This process will allow the identification of blowing agent mixtures for rigid polyurethane foams and represents a new area of endeavor in the search for third-generation blowing agents.

Appendix A. Commercial Availability of Blowing Agent Candidates

CAS #	Name	Availability
000591935	1,4-Pentadiene	Readily
123812806	3-Fluorocyclobutene	Not available
000142290	Cyclopentene	Readily
000563462	1-Butene, 2-methyl-	Readily
000504609	1,3-Pentadiene	Readily
000109671	1-Pentene	Readily
000109682	2-Pentene	Readily
000542927	1,3-Cyclopentadiene	Readily
000078795	1,3-Butadiene, 2-methyl-	Readily
000679867	1,1,2,2,3-Pentafluoropropane	HFC 245ca (Aldrich)
002366521	Butane, 1-fluoro-	Nar Chem
000513359	2-Butene, 2-methyl-	Readily
66	1,1,1,2,3-Pentafluoropropane	HFC 245eb
000558372	1-Butene, 3,3-dimethyl-	Readily
000374129	1,1,2,2-Tetrafluorocyclobutane	Columbia Organics
000461632	Difluoromethyl fluoromethyl ether	Synthesized by AEERL
345	1,1,2,3,4,4-Hexafluoro-1-butene	Not available
000107017	2-Butene	Readily
000078784	Butane, 2-methyl-	Readily
000691372	1-Pentene, 4-methyl-	Readily
6102	1,2-Difluorocyclobutane	Not known
6103	1,1-Difluorocyclobutane	Not known
000407590	1,1,1,4,4,4-Hexafluorobutane	HFC 356mff (Allied)
000666160	Fluorocyclobutane	Not known
000287923	Cyclopentane	Readily
6104	1,2,3-Trifluorocyclobutane	Not known
000677214	1-Propene, 3,3,3-trifluoro-	Aldrich
000287230	Cyclobutane	Readily
000460731	1,1,1,3,3-Pentafluoropropane	HFC 245fa Synthesized by AEERL
000067641	2-Propanone	Readily

Appendix A. Commercial Availability of Blowing Agent Candidates (continued)

CAS #	Name	Availability
000109660	Pentane	Readily
000421501	2-Propanone, 1,1,1-trifluoro	Aldrich
001115088	1,4-Pentadiene, 3-methyl-	Aldrich
6115	1,1-Difluorobutane	Not known
6117	1,4-Difluorobutane	Not available
001191964	Cyclopropane, ethyl-	Not known
333	1,2,3,4-Tetrafluorocyclobutane	Not known
000690222	Trifluoromethyl ethyl ether	Not available
6119	Trifluoromethoxymethoxymethane	Not known
000079298	Butane, 2,3-dimethyl-	Aldrich
6118	1,1,1-Trifluorobutane	Not available
000460435	1-Methoxy-2,2,2-trifluoroethane	Not known
001493034	Methane, iododifluoro-	Not known
000512516	1,1,2,2-Tetrafluoroethyl ethyl ether	Not known
000353617	Propane, 2-fluoro-2-methyl-	Not known
000503300	Trimethylene oxide	Aldrich
000594116	Cyclopropane, methyl-	Not known
6116	1,2-Difluorobutane	Not available
000680002	1,1,2,2,3,3-Hexafluoropropane	HFC 236ca
000109875	Dimethoxymethane	Aldrich
024270664	1,1,2,3,3-Pentafluoropropane	HFC 245ea
040723635	1,1,2,2-Tetrafluoropropane	Not known
000819498	1-Trifluoromethoxy-2-fluoroethane	Not known
6108	1,2,3-Trifluorocyclopentane	Not known
6101	1,1-Difluoroacetone	Not known
000382343	1,1,2,3,3,3-Pentafluoropropyl methyl ether	Not known
20	1,1,3,3-Tetrafluorooxetane	Synthesized by AEERL
000075763	Tetramethyl silane	Readily
000075832	Butane, 2,2-dimethyl-	Readily
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane	Not known

Appendix A. Commercial Availability of Blowing Agent Candidates (continued)

CAS #	Name	Availability
000421078	Propane, 1,1,1-trifluoro-	HFC 263fb
6107	1,2-Difluorocyclopentane	Not known
000431470	Methyl trifluoroacetate	Aldrich
6109	1,2,3,4-Tetrafluorocyclopentane	Not known
6105	Fluorocyclopentane	Not known
6106	1,1-Difluorocyclopentane	Not known
000075376	Ethane, 1,1-difluoro-	HFC 152a (Aldrich)
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-	Aldrich
6114	1,3-Difluoroacetone	Not known
000075105	Methane, difluoro-	HFC 32
032778168	1-Difluoromethoxy-2,2-difluoroethane	Not known
6111	1-Fluoro-2-ethylcyclopropane	Not known
069948294	1-Difluoromethoxy-1,1-difluoroethane	Not known
6112	1,1,1,3-Tetrafluoroacetone	Not known
123768183	1,1,2,2,3,3-Hexafluorocyclopentane	Not known
056281926	1-Difluoromethoxy-1,2,2-trifluoroethane	Not known
000360521	2-Propanone, 1,1,3,3-tetrafluoro	Not known
6110	2-Fluoroethylcyclopropane	Not known
000677565	1,1,1,2,2,3-Hexafluoropropane	HFC 236cb Synthesized by AEERL
000353366	Ethane, fluoro-	Should be available
001634044	t-Butyl methyl ether	Aldrich
000354643	Ethane, pentafluoroiodo-	Aldrich
000431710	2-Propanone, 1,1,1,3,3-pentafluoro	Not known
000811972	Ethane, 1,1,1,2-tetrafluoro-	HFC 134a (Aldrich)
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane	Not known
000373535	Methane, iodo fluoro-	Not known
000431630	1,1,1,2,3,3-Hexafluoropropane	HFC 236ea Synthesized by AEERL
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-	Not known
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-	Aldrich
032778113	1-Difluoromethoxy-1,1,2,2-tetrafluoroethane	Not known

Appendix A. Commercial Availability of Blowing Agent Candidates (continued)

CAS #	Name	Availability
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-	Aldrich
001691174	Difluoromethyl ether	Synthesized by AEERL
002314978	Methane, trifluoroiodo-	Aldrich
001814886	1,1,1,2,2-Pentafluoropropane	HFC 245cb Synthesized by AEERL
000382105	1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-	Not known
000690391	1,1,1,3,3,3-Hexafluoropropane	HFC 236fa
000333368	Bis-2,2,2-trifluoroethyl ether	Aldrich
000354336	Ethane, pentafluoro-	HFC 125
000421147	Trifluoromethyl methyl ether	Synthesized by AEERL
000931919	Hexafluorocyclopropane	Not known
18	1,1,2,2,3-Pentafluorooxetane	Synthesized by AEERL
002252848	1,1,1,2,2,3,3-Heptafluoropropane	HFC 227ca Synthesized by AEERL
000431890	1,1,1,2,3,3,3-Heptafluoropropane	HFC 227ea Synthesized by AEERL
444	2,3,4,5-Tetrafluorotetrahydrofuran	Not known
001479498	Trifluoromethyl ether	Synthesized by AEERL
003822682	Trifluoromethyl difluoromethyl ether	Synthesized by AEERL
000425821	1,1,2,2,3,3-Hexafluorooxetane	Synthesized by AEERL
000684162	2-Propanone, hexafluoro	Aldrich

Appendix B. Boiling Points of Blowing Agent Candidates at 760 mm Hg

CAS #	Name	BP (°C)	Reference
000067641	Acetone	56.00	Aldrich (1994)
000075105	Methane, difluoro-	-51.65	Yu-halada, LC. and Reichel, C.J. (1993)
000075376	Ethane, 1,1-difluoro-	-25.00	Aldrich (1994)
000075763	Tetramethyl silane	26.00	Aldrich (1994)
000075832	Butane, 2,2-dimethyl-	50.00	Aldrich (1994)
000078784	Butane, 2-methyl-	28.00	Aldrich (1994)
000079298	Butane, 2,3-dimethyl-	58.00	Aldrich (1994)
000107017	2-Butene	1.00	Aldrich (1994)
000109660	Pentane	36.10	Aldrich (1994)
000109671	1-Pentene	29.90	Aldrich (1994)
000109682	2-Pentene	37.00	Aldrich (1994)
000109875	Dimethoxymethane	41.00	Aldrich (1994)
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-	-28.00	Aldrich (1994)
000142290	Cyclopentene	44.00	Aldrich (1994)
000287230	Cyclobutane	12.50	Daubert, TE. and Danner, RP. (1989)
000287923	Cyclopentane	50.00	Aldrich (1994)
000333368	Bis-2,2,2-trifluoroethyl ether	9.50	
000353366	Ethane, fluoro-	-37.70	Daubert, TE. and Danner, RP. (1989)
000353617	Propane, 2-fluoro-2-methyl-	-5.02	
000354336	Ethane, pentafluoro-	-48.50	Creazzo, JA. and Hammel, HS. (1991)
000354643	Ethane, pentafluoroiodo-	12.00	Nimitz, J. and Lankford, PW. (1993)
000360521	2-Propanone, 1,1,3,3-tetrafluoro	23.31	
000372907	1,4-Difluorobutane	28.82	
000373535	Methane, iodofluoro-	53.40	Nimitz, J. and Lankford, PE. (1993)
000374129	1,1,2,2-Tetrafluorocyclobutane	0.76	
000382105	1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-	-29.10	
000382343	1,1,2,3,3,3-Pentafluoropropyl methyl ether	-7.07	
000407590	1,1,1,4,4,4-Hexafluorobutane	24.90	Knopeck, GM. et al. (1993)
000421078	Propane, 1,1,1-trifluoro-	-13.00	Decaire, BR. et al. (1992)
000421147	Trifluoromethyl methyl ether	-24.10	Smith, ND. (1993)
000421501	2-Propanone, 1,1,1-trifluoro	26.21	
000425821	1,1,2,2,3,3-Hexafluorooxetane	-28.20	Smith, ND. (1993)
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane	-12.54	
000431050	1,1-Difluoroacetone	34.13	
000431312	1,1,1,2,3-Pentafluoropropane	22.70	
000431470	Methyl trifluoroacetate	43.00	Aldrich (1994)
000431630	1,1,1,2,3,3-Hexafluoropropane	6.00	Decaire, BR. et al. (1992)
000431710	2-Propanone, 1,1,1,3,3-pentafluoro	15.28	
000431890	1,1,1,2,3,3,3-Heptafluoropropane	-18.70	Decaire, BR. et al. (1992)
000453145	1,3-Difluoroacetone	49.87	
000460344	1,1,1-Trifluorobutane	0.38	
000460435	1-Methoxy-2,2,2-trifluoroethane	1.45	
000460731	1,1,1,3,3-Pentafluoropropane	15.30	Knopeck, GM. et al. (1993)
000461632	Difluoromethyl fluoromethyl ether	29.90	
000503300	Trimethylene oxide	50.00	Aldrich (1994)
000512516	1,1,2,2-Tetrafluoroethyl ethyl ether	14.95	
000513359	2-Butene, 2-methyl-	35.00	Aldrich (1994)
000558372	1-Butene, 3,3-dimethyl-	41.00	Aldrich (1994)
000563462	1-Butene, 2-methyl-	31.00	Aldrich (1994)
000591935	1,4-Pentadiene	26.00	Aldrich (1994)
000594116	Cyclopropane, methyl-	4.00	

Appendix B. Boiling Points of Blowing Agent Candidates at 760 mm Hg (continued)

CAS #	Name	BP (°C)	Reference
000666160	Fluorocyclobutane	29.19	
000677214	1-Propene, 3,3,3-trifluoro-	-18.00	Aldrich (1994)
000677565	1,1,1,2,2,3-Hexafluoropropane	-1.20	Decaire, BR. et al. (1992)
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-	38.00	Nimitz, J. and Lankford, PE. (1993)
000679867	1,1,2,2,3-Pentafluoropropane	25.10	Decaire, BR. et al. (1992)
000680002	1,1,2,2,3,3-Hexafluoropropane	10.00	Decaire, BR. et al. (1992)
000680546	1,1,2,3,4,4-Hexafluoro-1-butene	-3.77	
000684162	2-Propanone, hexafluoro	-26.00	Aldrich (1994)
000686657	1,2-Difluorobutane	8.56	
000690222	Trifluoromethyl ethyl ether	1.45	
000690391	1,1,1,3,3,3-Hexafluoropropane	-0.07	Decaire, BR. et al. (1992)
000691372	1-Pentene, 4-methyl-	53.00	Aldrich (1994)
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-	40.00	Nimitz, J. and Lankford, PE. (1993)
000811972	Ethane, 1,1,1,2-tetrafluoro-	-26.50	Decaire, BR. et al. (1992)
000819498	1-Trifluoromethoxy-2-fluoroethane	4.14	
000931919	Hexafluorocyclopropane	-47.70	
001115088	1,4-Pentadiene, 3-methyl-	55.00	Aldrich (1994)
001120203	1,1-Difluorocyclopentane	46.57	
001191964	Cyclopropane, ethyl-	34.50	
001479498	Trifluoromethyl ether	-58.70	Smith, ND. (1993)
001481363	Fluorocyclopentane	57.64	
001493034	Methane, iododifluoro-	21.60	Nimitz, J. and Lankford, PE. (1993)
001634044	t-Butyl methyl ether	55.00	Aldrich (1994)
001691174	Difluoromethyl ether	4.70	Smith, ND. (1993)
001814886	1,1,1,2,2-Pentafluoropropane	-17.60	Decaire, BR. et al. (1992)
002252848	1,1,1,2,2,3,3-Heptafluoropropane	-17.70	Decaire, BR. et al. (1992)
002314978	Methane, trifluoroiodo-	-22.50	Nimitz, J. and Lankford, PE. (1993)
002358385	1,1-Difluorobutane	8.56	
002366521	Butane, 1-fluoro-	32.50	
003822682	Trifluoromethyl difluoromethyl ether	-34.60	Smith, ND. (1993)
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-	41.00	Nimitz, J. and Lankford, PE. (1993)
022669096	1,1-Difluorocyclobutane	17.69	
024270664	1,1,2,3,3-Pentafluoropropane	39.30	Knopeck, GM. et al. (1993)
032778113	1-Difluoromethoxy-1,1,2,2-tetrafluoroethane	-3.10	Smith, ND. (1993)
032778168	1-Difluoromethoxy-2,2-difluoroethane	-1.54	
040723635	1,1,2,2-Tetrafluoropropane	-1.60	Decaire, BR. et al. (1992)
050422769	1-Fluoro-2-ethylcyclopropane	45.44	
056281926	1-Difluoromethoxy-1,2,2-trifluoroethane	-15.58	
069750681	2-Fluoroethylcyclopropane	52.94	
069948294	1-Difluoromethoxy-1,1-difluoroethane	-12.54	
072507858	1,2-Difluorocyclobutane	24.07	
113742908	1,2-Difluorocyclopentane	52.71	
123768183	1,1,2,2,3,3-Hexafluorocyclopentane	13.58	
123812806	3-Fluorocyclobutene	32.67	
129362976	1,2,3,4-Tetrafluorocyclobutane	13.74	
133360006	2,3,4,5-Tetrafluorotetrahydrofuran	49.77	
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane	9.73	
144109035	1,1,2,2,3-Pentafluorooxetane	3.40	Smith, ND. (1993)
154330402	1,1,3,3-Tetrafluorooxetane	21.20	Smith, ND. (1993)
6104	1,2,3-Trifluorocyclobutane	18.92	
6108	1,2,3-Trifluorocyclopentane	47.75	
6109	1,2,3,4-Tetrafluorocyclopentane	42.76	

Appendix B. Boiling Points of Blowing Agent Candidates at 760 mm Hg (continued)

CAS #	Name	BP (°C)	Reference
6112	1,1,1,3-Tetrafluoroacetone	28.81	
6119	Trifluoromethoxymethoxymethane	29.52	

Appendix C. Physical Properties of Blowing Agent Candidates I - Environmental Fate

CAS No.	Name	MP	WS	Tmp	Kow	VP	Tmp	HL	Tmp
000067641	2-Propanone	-94.70	1e6	25	-0.24	230.00	25		
000075105	Methane, difluoro-	-136.00			2.00E-01	12,600.00	25		
000075376	Ethane, 1,1-difluoro-	-117.00			7.50E-01	4,437.10	25		
000075763	Tetramethyl silane	-99.00	1.96	25	3.85	718.00	25		
000075832	Butane, 2,2-dimethyl-	-100.00	18	25	3.82E+00	320.00	25		
000078784	Butane, 2-methyl-	-159.90	4.80E+01	25	2.30E+00	689.00	25	1.40E+00	25
000079298	Butane, 2,3-dimethyl-	-129.00	11	20	3.85E+00	235.00	25		
000107017	2-Butene	-140.00			2.33E+00	1,360.00	20	1.54E-01	25
000109660	Pentane	-130.00	3.80E+01	25	3.39E+00	514.00	25	1.25E+00	25
000109671	1-Pentene	-165.22	148	25		638.00	25		
000109682	2-Pentene	-138.00	203	25		528.00	25		
000109875	Dimethoxymethane	-105.15	244	16		398.70	25		
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-	-153.00				4,900.00	25		
000142290	Cyclopentene	-135.00				380.00	25		
000287230	Cyclobutane	-91.00				1,170.00	25		
000287923	Cyclopentane	-94.40	1.56E+02	25	3.00E+00	318.00	25	1.88E-01	25
000333368	Bis-2,2,2-trifluoroethyl ether								
000353366	Ethane, fluoro-	-143.00				6,840.00	25		
000353617	Propane, 2-fluoro-2-methyl-								
000354336	Ethane, pentafluoro-	-103.00	3.90E+01	25	1.43E+00	10,499.00	25	3.05E+00	25
000354643	Ethane, pentafluoroiodo-	-95.00				717.00	10		
000360521	2-Propanone, 1,1,3,3-tetrafluoro								
000372907	1,4-Difluorobutane								
000373535	Methane, iodo fluoro-								
000374129	1,1,2,2-Tetrafluorocyclobutane								
000382105	1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-								
000382343	1,1,2,3,3,3-Pentafluoropropyl methyl ether								
000407590	1,1,1,4,4,4-Hexafluorobutane								
000421078	Propane, 1,1,1-trifluoro-								
000421147	Trifluoromethyl methyl ether								
000421501	2-Propanone, 1,1,1-trifluoro								
000425821	1,1,2,2,3,3-Hexafluorooxetane								
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane								
000431050	1,1-Difluoroacetone								
000431312	1,1,1,2,3-Pentafluoropropane								
000431470	Methyl trifluoroacetate								
000431630	1,1,1,2,3,3-Hexafluoropropane	-146.10							
000431710	2-Propanone, 1,1,1,3,3-pentafluoro								
000431890	1,1,1,2,3,3,3-Heptafluoropropane								
000453145	1,3-Difluoroacetone								
000460344	1,1,1-Trifluorobutane								
000460435	1-Methoxy-2,2,2-trifluoroethane								

MP = Melting Point in °C

WS = Water solubility in mg/kg

Tmp = Temperature in °C

Kow = Log octanol/water partition coefficient

VP = Vapor pressure in mm hg

HL = Henry's Law constant in atm cu-m/mole

Appendix C. Physical Properties of Blowing Agent Candidates I - Environmental Fate (continued)

CAS No.	Name	MP	WS	Tmp	Kow	VP	Tmp	HL	Tmp
000460731	1,1,1,3,3-Pentafluoropropane								
000461632	Difluoromethyl fluoromethyl ether								
000503300	Trimethylene oxide					324.00	25		
000512516	1,1,2,2-Tetrafluoroethyl ethyl ether								
000513359	2-Butene, 2-methyl-	-134.00				610.00	25		
000558372	1-Butene, 3,3-dimethyl-	-115.00				430.00	25		
000563462	1-Butene, 2-methyl-	-137.00				610.00	25		
000594116	Cyclopropane, methyl-								
000666160	Fluorocyclobutane								
000677214	1-Propene, 3,3,3-trifluoro-								
000677565	1,1,1,2,2,3-Hexafluoropropane								
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-								
000679867	1,1,2,2,3-Pentafluoropropane	-73.40							
000680002	1,1,2,2,3,3-Hexafluoropropane								
000680546	1,1,2,3,4,4-Hexafluoro-1-butene								
000684162	2-Propanone, hexafluoro					5,074.00	25		
000686657	1,2-Difluorobutane								
000690222	Trifluoromethyl ethyl ether								
000690391	1,1,1,3,3,3-Hexafluoropropane								
000691372	1-Pentene, 4-methyl-	-153.00				271.00	25		
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-	-95.00							
000811972	Ethane, 1,1,1,2-tetrafluoro-	-101.00	6.70E+01	25	1.27E+00	430.00	25	1.53E+00	25
000819498	1-Trifluoromethoxy-2-fluoroethane								
000931919	Hexafluorocyclopropane								
001115088	1,4-Pentadiene, 3-methyl-								
001120203	1,1-Difluorocyclopentane								
001191964	Cyclopropane, ethyl-								
001479498	Trifluoromethyl ether								
001481363	Fluorocyclopentane								
001493034	Methane, iododifluoro-								
001634044	t-Butyl methyl ether	-115.00	51000	25	1.24	249.00	25		
001691174	Difluoromethyl ether								
001814886	1,1,1,2,2-Pentafluoropropane								
002252848	1,1,1,2,2,3,3-Heptafluoropropane								
002314978	Methane, trifluoroiodo-					4,395.00	20		
002358385	1,1-Difluorobutane								
002366521	Butane, 1-fluoro-				2.00E+00				
003822682	Trifluoromethyl difluoromethyl ether								
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-								
022669096	1,1-Difluorocyclobutane								
024270664	1,1,2,3,3-Pentafluoropropane								
032778113	1-Difluoromethoxy-1,1,2,2-tetrafluoroethane								

MP = Melting Point in °C

WS = Water solubility in mg/kg

Tmp = Temperature in °C

Kow = Log octanol/water partition coefficient

VP = Vapor pressure in mm hg

HL = Henry's Law constant in atm cu-m/mole

Appendix C. Physical Properties of Blowing Agent Candidates I - Environmental Fate (continued)

CAS No.	Name	MP	WS	Tmp	Kow	VP	Tmp	HL	Tmp
032778168	1-Difluoromethoxy-2,2-difluoroethane								
040723635	1,1,2,2-Tetrafluoropropane								
050422769	1-Fluoro-2-ethylcyclopropane								
056281926	1-Difluoromethoxy-1,2,2-trifluoroethane								
069750681	2-Fluoroethylcyclopropane								
069948294	1-Difluoromethoxy-1,1-difluoroethane								
072507858	1,2-Difluorocyclobutane								
113742908	1,2-Difluorocyclopentane								
123768183	1,1,2,2,3,3-Hexafluorocyclopentane								
123812806	3-Fluorocyclobutene								
129362976	1,2,3,4-Tetrafluorocyclobutane								
133360006	2,3,4,5-Tetrafluorotetrahydrofuran								
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane								
144109035	1,1,2,2,3-Pentafluorooxetane								
154330402	1,1,3,3-Tetrafluorooxetane								
6104	1,2,3-Trifluorocyclobutane								
6108	1,2,3-Trifluorocyclopentane								
6109	1,2,3,4-Tetrafluorocyclopentane								
6112	1,1,1,3-Tetrafluoroacetone								
6119	Trifluoromethoxymethoxymethane								

MP = Melting Point in °C

WS = Water solubility in mg/kg

Tmp = Temperature in °C

Kow = Log octanol/water partition coefficient

VP = Vapor pressure in mm hg

HL = Henry's Law constant in atm cu-m/mole

Appendix D. Physical Properties of Blowing Agent Candidates II - Environmental Fate

CAS No.	Name	SpecGrav	tmp	HeatVap	tmp	Flash Pt	Meth	LEL	UEL
000067641	2-Propanone	0.79		7.48	25	-9.00	TOC		
000075105	Methane, difluoro-					-89.00			27.2
000075376	Ethane, 1,1-difluoro-	0.91	20	4.561	25				
000075763	Tetramethyl silane	0.65		5.785	26	-27.00		1.5	6
000075832	Butane, 2,2-dimethyl-	0.64	25	6.618	25	-34.00	TCC		
000078784	Butane, 2-methyl-	0.61	25	5.937	25	-57.00	CC		
000079298	Butane, 2,3-dimethyl-	0.66	25	6.961	25	-33.00	TCC		
000107017	2-Butene					-30.00	TCC		
000109660	Pentane	0.62	25	6.32	25	-40.00	TOC	1.5	7.8
000109671	1-Pentene	0.64	25	6.088	25	-28.00	TCC		
000109682	2-Pentene	0.65	25	8.42	25	-45.00	TCC		
000109875	Dimethoxymethane	0.85	15	60904	25				
000116154	1-Propene, 1,1,2,3,3,3-hexafluoro-								
000142290	Cyclopentene	0.77	25			-34.00	TCC	1.5	12.1
000287230	Cyclobutane					-64.00		1.8	11.1
000287923	Cyclopentane	0.74	25	6.808	25	-37.00			
000333368	Bis-2,2,2-trifluoroethyl ether								
000353366	Ethane, fluoro-					-89.00			17.3
000353617	Propane, 2-fluoro-2-methyl-								
000354336	Ethane, pentafluoro-					-28.00			
000354643	Ethane, pentafluoroiodo-	2.09							
000360521	2-Propanone, 1,1,3,3-tetrafluoro								
000372907	1,4-Difluorobutane								
000373535	Methane, iodo fluoro-	2.37							
000374129	1,1,2,2-Tetrafluorocyclobutane								
000382105	1-Propene, 3,3,3-trifluoro-2-(trifluoromethyl)-								
000382343	1,1,2,3,3,3-Pentafluoropropyl methyl ether								
000407590	1,1,1,4,4,4-Hexafluorobutane								
000421078	Propane, 1,1,1-trifluoro-								
000421147	Trifluoromethyl methyl ether								
000421501	2-Propanone, 1,1,1-trifluoro	1.25				-23.00	TCC		
000425821	1,1,2,2,3,3-Hexafluoroacetone								
000425887	1-Methoxy-1,1,2,2-tetrafluoroethane								
000431050	1,1-Difluoroacetone								
000431312	1,1,1,2,3-Pentafluoropropane								
000431470	Methyl trifluoroacetate								
000431630	1,1,1,2,3,3-Hexafluoropropane	1.39						0	0
000431710	2-Propanone, 1,1,1,3,3-pentafluoro								
000431890	1,1,1,2,3,3,3-Heptafluoropropane								
000453145	1,3-Difluoroacetone								

SpecGrav = Specific gravity

tmp = Temperature in degrees C

HeatVap = Heat of Vaporization in cal/g

Flash Pt = Flash point in degrees C

Meth = Flash point method

LEL = Lower explosion limit

UEL = Upper explosion limit

Appendix D. Physical Properties of Blowing Agent Candidates II - Environmental Fate (continued)

CAS No.	Name	SpecGrav	tmp	HeatVap	tmp	Flash Pt	Meth	LEL	UEL
000460344	1,1,1-Trifluorobutane								
000460435	1-Methoxy-2,2,2-trifluoroethane								
000460731	1,1,1,3,3-Pentafluoropropane								
000461632	Difluoromethyl fluoromethyl ether								
000503300	Trimethylene oxide	0.89				-28.00	TCC	2.8	37
000512516	1,1,2,2-Tetrafluoroethyl ethyl ether								
000513359	2-Butene, 2-methyl-	0.66				-45.00	TCC	1.4	9.6
000558372	1-Butene, 3,3-dimethyl-	0.65				-28.00	TCC	1.2	9.0
000563462	1-Butene, 2-methyl-	0.65				-34.00	TCC		
000594116	Cyclopropane, methyl-								
000666160	Fluorocyclobutane								
000677214	1-Propene, 3,3,3-trifluoro-								
000677565	1,1,1,2,2,3-Hexafluoropropane								
000677690	Propane, 1,1,1,2,3,3,3-heptafluoro-2-iodo-	2.10							
000679867	1,1,2,2,3-Pentafluoropropane	1.34						0	0
000680002	1,1,2,2,3,3-Hexafluoropropane								
000680546	1,1,2,3,4,4-Hexafluoro-1-butene								
000684162	2-Propanone, hexafluoro								
000686657	1,2-Difluorobutane								
000690222	Trifluoromethyl ethyl ether								
000690391	1,1,1,3,3,3-Hexafluoropropane								
000691372	1-Pentene, 4-methyl-	0.67				-31.00	TCC	1.2	9.4
000754347	Propane, 1,1,1,2,2,3,3-heptafluoro-3-iodo-	2.06	.11						
000811972	Ethane, 1,1,1,2-tetrafluoro-								
000819498	1-Trifluoromethoxy-2-fluoroethane								
000931919	Hexafluorocyclopropane								
001115088	1,4-Pentadiene, 3-methyl-	0.67				-34.00	TCC		
001120203	1,1-Difluorocyclopentane								
001191964	Cyclopropane, ethyl-								
001479498	Trifluoromethyl ether								
001481363	Fluorocyclopentane								
001493034	Methane, iododifluoro-	3.24							
001634044	t-Butyl methyl ether	0.74				-10.00	TCC		
001691174	Difluoromethyl ether								
001814886	1,1,1,2,2-Pentafluoropropane								
002252848	1,1,1,2,2,3,3-Heptafluoropropane								
002314978	Methane, trifluoroiodo-	2.36	.038						
002358385	1,1-Difluorobutane								
002366521	Butane, 1-fluoro-								
003822682	Trifluoromethyl difluoromethyl ether								

SpecGrav = Specific gravity

tmp = Temperature in degrees C

HeatVap = Heat of Vaporization in cal/g

Flash Pt = Flash point in degrees C

Meth = Flash point method

LEL = Lower explosion limit

UEL = Upper explosion limit

Appendix D. Physical Properties of Blowing Agent Candidates II - Environmental Fate (continued)

CAS No.	Name	SpecGrav	tmp	HeatVap	tmp	Flash Pt	Meth	LEL	UEL
003831490	Ethane, 1-iodo-1,1,2,2-tetrafluoro-								
022669096	1,1-Difluorocyclobutane								
024270664	1,1,2,3,3-Pentafluoropropane								
032778113	1-Difluoromethoxy-1,1,2,2-tetrafluoroethane								
032778168	1-Difluoromethoxy-2,2-difluoroethane								
040723635	1,1,2,2-Tetrafluoropropane								
050422769	1-Fluoro-2-ethylcyclopropane								
056281926	1-Difluoromethoxy-1,2,2-trifluoroethane								
069750681	2-Fluoroethylcyclopropane								
069948294	1-Difluoromethoxy-1,1-difluoroethane								
072507858	1,2-Difluorocyclobutane								
113742908	1,2-Difluorocyclopentane								
123768183	1,1,2,2,3,3-Hexafluorocyclopentane								
123812806	3-Fluorocyclobutene								
129362976	1,2,3,4-Tetrafluorocyclobutane								
133360006	2,3,4,5-Tetrafluorotetrahydrofuran								
136975092	1-Trifluoromethyl-1,2,2-trifluorocyclobutane								
144109035	1,1,2,2,3-Pentafluorooxetane								
154330402	1,1,3,3-Tetrafluorooxetane								
6104	1,2,3-Trifluorocyclobutane								
6108	1,2,3-Trifluorocyclopentane								
6109	1,2,3,4-Tetrafluorocyclopentane								
6112	1,1,1,3-Tetrafluoroacetone								
6119	Trifluoromethoxymethoxymethane								

SpecGrav = Specific gravity
 tmp = Temperature in degrees C
 HeatVap = Heat of Vaporization in cal/g
 Flash Pt = Flash point in degrees C
 Meth = Flash point method
 LEL = Lower explosion limit
 UEL = Upper explosion limit

Appendix E. References for Experimental Physical Properties from Appendices C and D

CAS No.	Ref MP	Ref WS	Ref Kow	Ref VP	Ref HL	Ref SG	Ref HV	Ref FP	Ref EL
000067641	RIDDI	RIDDI	H&L	DD		ALDRI	RIDDI	RIDDI	
000075105	DD		H&L	DD				DD	DD
000075376	ALDRI		H&L	RIDDI		RIDDI	RIDDI		
000075763	ALDRI	RIDDI	H&L	DD		ALDRI	RIDDI	DD	DD
000075832	ALDRI	RIDDI	H&L	RIDDI		RIDDI	RIDDI	ALDRI	
000078784	RIDDI	RIDDI	H&L	DD		RIDDI	RIDDI	RIDDI	
000079298	ALDRI	RIDDI	H&L	DD		RIDDI	RIDDI	ALDRI	
000107017	ALDRI		H&L	OB				ALDRI	
000109660	ALDRI	RIDDI	H&L	DD		RIDDI	RIDDI	RIDDI	
000109671	RIDDI	RIDDI		RIDDI		RIDDI	RIDDI	ALDRI	
000109682	RIDDI	RIDDI		RIDDI		RIDDI	RIDDI	ALDRI	
000109875	RIDDI	RIDDI		RIDDI		RIDDI	RIDDI		
000116154	ALDRI			DD					
000142290	ALDRI			DD		ALDRI		ALDRI	DD
000287230	DD			DD				DD	DD
000287923	ALDRI	YA	H&L	DD		RIDDI	RIDDI	RIDDI	
000333368									
000353366	DD			DD				DD	DD
000353617									
000354336	DD			DD				DD	
000354643	IKON			IKON		IKON			
000360521									
000372907									
000373535						IKON			
000374129									
000382105									
000382343									
000407590									
000421078									
000421147									
000421501						ALDRI		ALDRI	
000425821									
000425887									
000431050									
000431312									
000431470									
000431630									
000431710									
000431890									
000453145									
000460344									
000460435									

ALDRI = Aldrich (1994); DD = Daubert and Danner (1989); H&L = Hansch and Leo (1985)
 IKON = Lankford, PE., and Nimitz, J. (1993); Riddi = Riddick, JA. et al. (1986)
 OB = Obenaus, F. et al. (1985); YK = Yalkowsky, SH. et al (1987)
 BE = Bennet, GM. and Phillip, WG. (1928); FU = Fujiwara, Y. et al. (1984)

Appendix E. References for Experimental Physical Properties from Appendices C and D (continued)

CAS No.	Ref MP	Ref WS	Ref Kow	Ref VP	Ref HL	Ref SG	Ref HV	Ref FP	Ref EL
000460731									
000461632									
000503300				DD		ALDRI		ALDRI	DD
000512516									
000513359	ALDRI			DD		ALDRI		ALDRI	DD
000558372	ALDRI			DD		ALDRI		ALDRI	DD
000563462	ALDRI			DD		ALDRI		ALDRI	
000594116									
000666160									
000677214									
000677565									
000677690						IKON			
000679867									
000680002									
000680546									
000684162				DD					
000686657									
000690222									
000690391									
000691372	DD			DD		ALDRI		ALDRI	DD
000754347						IKON	IKON		
000811972									
000819498									
000931919									
001115088						ALDRI		ALDRI	
001120203									
001191964									
001479498									
001481363									
001493034						IKON			
001634044	ALDRI	BE	FU	DD		ALDRI		ALDRI	
001691174									
001814886									
002252848									
002314978				IKON		IKON			
002358385									
002366521			H&L						
003822682									
003831490									
022669096									
024270664									
032778113									

ALDRI = Aldrich (1994); DD = Daubert and Danner (1989); H&L = Hansch and Leo (1985)
 IKON = Lankford, PE., and Nimitz, J. (1993); Riddi = Riddick, JA. et al. (1986)
 OB = Obenaus, F. et al. (1985); YK = Yalkowsky, SH. et al. (1987)
 BE = Bennet, GM. and Phillip, WG. (1928); FU = Fujiwara, Y. et al. (1984)

Appendix E. References for Experimental Physical Properties from Appendices C and D (continued)

CAS No.	Ref MP	Ref WS	Ref Kow	Ref VP	Ref HL	Ref SG	Ref HV	Ref FP	Ref EL
032778168									
040723635									
050422769									
056281926									
069750681									
069948294									
072507858									
113742908									
123768183									
123812806									
129362976									
133360006									
136975092									
144109035									
154330402									
6104									
6108									
6109									
6112									
6119									

ALDRI = Aldrich (1994); DD = Daubert and Danner (1989); H&L = Hansch and Leo (1985)
 IKON = Lankford, PE., and Nimitz, J. (1993); Riddi = Riddick, JA. et al. (1986)
 OB = Obenaus, F. et al. (1985); YK = Yalkowsky, SH. et al (1987)
 BE = Bennet, GM. and Phillip, WG. (1928); FU = Fujiwara, Y. et al. (1984)

References

- Aldrich. Aldrich Catalog Handbook of Fine Chemicals. Aldrich Chemical Company, Milwaukee, WI. (1994).
- ASTM. Provisional Standard under Development for CF₃I. ASTM Standardization News. December 16 (1994).
- Atkinson, R. Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds under Atmospheric Conditions. Chem. Rev. 85, 69-201 (1985).
- Atkinson, R. Gas-Phase Tropospheric Chemistry of Organic Compounds. J. Phys. Chem. Ref. Monog. 2, 1-216 (1994).
- Ball, EE. and Lamberts, WM. HFC 356, a Zero ODP Blowing Agent Candidate for North American Appliance Foam Formulations. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 10-13 (1993).
- Ballhaus, H. and Hahn, H. Hydrocarbons Provide Zero ODP and Zero GWP Insulation for Household Refrigeration. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 33-39 (1993).
- Barthelemy, PP., Leroy, A., Franklin, JA., Zipfel, L., and Krucke, W. Blowing Agents for Rigid Polyurethane Foams Using Conventional Dispensing Equipment. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 14-21 (1993).
- Bennett, GM. and Phillip, WG. The Influence of Structure on the Solubility of Ethers. Part I. Aliphatic Ethers. J. Chem Soc, 1930-7 (1928).
- Bosch, SJ. and Basu, DK. Revised and Updated Drinking Water Quantification of Toxicological Effects for Methyl *tert*-Butyl Ether. Syracuse Research Corporation. Cincinnati, OH. Prepared for Environmental Criteria and Assessment Office, US EPA (1992).
- Budavari, S., O'Neil, MJ., Smith, A., and Heckelman, PE. The Merck Index. Eleventh Edition. Merck and Co., Inc., Rahway, NJ (1989).
- C&E News, News Focus: Chemical Arms Treaty Makes Unprecedented Demands of Industry. Chem. Eng. News, June 7, pp 7-18 (1993).
- Cecchini, C., Cellarosi, B., Cancellier, V., and Pirotta, GP. Alternative Blowing Agents for CFC Rigid PU Foams. Proceedings of the Polyurethanes World Congress, 1991. Technomic Publishing Co., Lancaster, PA, 720-7 (1991).
- Cecchini, C., Cancellier, V., and Cellarosi, B. Employment of Zero ODP Blowing Agents for Polyurethane Rigid Foams for Thermal Insulation. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 354-60 (1993).

Chemeides, WL. and Davis, DD. Iodine, Its Possible Role in Tropospheric Photochemistry. *J. Geophys. Res.*, 85, 7383-98 (1980).

Chemical Marketing Reporter. Potential Drawback Found for HFCs. July 4, p 7 (1994).

Creazzo, JA., and Hammel, HS. Replacing CFC-11 with HCFC-22 in Proceedings of the Polyurethanes World Congress, 1991. Technomic Publishing Co., Lancaster, PA, 214-9 (1991).

Creazzo, JA., Hammel, HS., Schindler, P., and Cicalo, KJ. Zero-ODP Blowing Agents for Polyurethane Foam. In Polyurethane Foams. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 456-64 (1993).

Daubert, TE. and Danner, RP. Physical and Thermodynamic Properties of Pure Chemicals. Design Institute for Physical Property Data. American Institute of Chemical Engineers, Taylor and Francis Publishing, Washington, DC (1989).

Dcaire, BR., Pham, HT., Richard, RG., and Shankland, IR. Blowing Agents, the Next Generation. Polyurethanes 92. Proceedings of the Society of the Plastics Industry 34th Annual Technical/Marketing Conference. 1992. Technomic Publishing Co., Lancaster, PA, 2-11 (1992).

ES&T. ES&T Currents. *Environ. Sci. Technol.*, 28(4), 171A (1994).

Falbe, J., Lappe, P., and Weber, J. Aldehydes, Aliphatic and Aromatic in Ullmann's Encyclopedia of Industrial Chemistry. VCH Publishers, New York, NY. Vol A1, pp 321-352 (1985).

Fujiwara, Y., Kinoshita, T., Sato, H., and Kojima, I. Biodegradation and Bioconcentration of Alkyl Ethers. *Yukagaku*, 33, 111-14 (1984).

Griesbaum, K., Honicke, D., and Olson, M. Cyclopentadiene and Cyclopentene in Ullmann's Encyclopedia of Industrial Chemistry. VCH Publishers, New York, NY. Vol A8, pp 227-37 (1987).

Griesbaum, K., Behr, A., Didenkapp, D., Voges, H., Garbe, D., Paetz, C., Collin, G., Mayer, D., and Hoke, H. Hydrocarbons in Ullmann's Encyclopedia of Industrial Chemistry. VCH Publishers, New York, NY. Vol A13, pp 227-281 (1989).

Hansch, C., and Leo, A. MEDCHEM Project. Pomona College. Claremont, CA. (1985)

Heilig, G. and Wiedermann, RE. Pentane Blown Polyurethane Rigid Foams for Construction. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 241-6 (1993).

Howard, PH., Sage, GW., Lamacchia, A., and Colb, A. The Development of an Environmental Fate Data Base. *J. Chem. Inf. Comput. Sci.*, 22, 38-44 (1982).

- Howard, PH., Hueber, AE., Mulesky, BC., Crisman, JS., Meylan, W., Crosbie, E., Gray, DA., Sage, GW., Howard, KP., LaMacchia, A., Boethling, B., and Trost, R. BIOLOG, BIODEG and FATE/EXPOS: New Files on Microbial Degradation of Toxicity as well as Environmental Fate/Exposure of Chemicals. *Environ. Tox. Chem.*, 5, 977-88 (1986).
- Joback, KG. MS. thesis, MIT, Cambridge, MA, June (1982).
- Kaufman, CM. and Overcash, MR. Green Biomass Materials in Polyurethane Foams. *Air & Waste*, 43, 1253-9 (1993).
- Kennedy, GL. Toxicology of Fluorine-Containing Monomers. *Crit. Rev. Tox.*, 21, 149-70 (1990).
- Kiem, W. and Roper, M. Acylation and Alkylation in Ullmann's Encyclopedia of Industrial Chemistry. VCH Publishers, New York, NY. Vol A1, pp 185-220 (1985).
- Knopeck, GM., Parker, RC., Richard, RG., and Shankland, IR. Evaluation of Next Generation Blowing Agents. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 465-72 (1993).
- Krauss, R. and Stephan, K. Thermal Conductivity of Refrigerants in a Wide Range of Temperature and Pressure. *J. Phys. Chem. Ref. Data.*, 16, 43-77 (1969).
- Kuhn, E. and Schindler, P. Advances in the Understanding of the Effects of Various Blowing Agents on Rigid Polyurethane Appliance Foam Properties. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 22-28 (1993).
- Lankford, PE. and Nimitz, J. New Class of High-Performance, Environmentally Sound Refrigerants. International CFC and Halon Alternatives Conference, Washington, D.C., Oct 20-22 (1993).
- Meylan, WM. and Howard, PH. Bond contribution method for estimating Henry's law constants. *Environ.Toxic.Chem.* 10:1283-93 (1991).
- Meylan, W.M. and Howard, PH. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* 12: 2293-2299 (1993).
- Missenard, FA. Thermal Conductivity of Pure Gases at Different Temperatures and Pressures. *RGT*, 50: 125-37 (1966).
- Nimitz, J. and Lankford, PE. Fluoroiodocarbons as Halon Replacements. International CFC and Halon Alternatives Conference, Washington, D.C., Oct 20-22 (1993).
- Obenaus, F., Droste, W., Neumeister, J., and Huls, AG. Butenes in Ullmann's Encyclopedia of Industrial Chemistry. Gerhartz, G. Ed. VCH Publishing Co., Deerfield Beach, FL. Vol A4, pp 483-94 (1985).

- Rasmussen, RA., Khalil, MAK., Gunawardena, R., and Hoyt, SD. Atmospheric Methyl Iodide (CH_3). *J. Geophys. Res.* 87, 3086-90 (1982).
- Ravishankara, AR., Solomon, S., Turnipseed, AA., and Warren, R.F. Atmospheric Lifetimes of Long-Lived Halogenated Species. *Science*, 259, 194-199 (1993).
- Ravishankara, AR., Andrew, AT., Jensen, NR., Barone, S., Mills, M., Howard, CJ., and Solomon, S. Do Hydrofluorocarbons Destroy Stratospheric Ozone? *Science*, 263, 71-5 (1994).
- Reid, RC., Prausnitz, JM., and Poling, BE. *The Properties of Gases and Liquids*. Fourth Edition. McGraw Hill Inc., New York, NY. (1987).
- Riddick, JA., Bunger, WB., and Sakano, TK. *Techniques of Chemistry, Vol II, Organic Solvents*. John Wiley & Sons, New York, NY (1986).
- Roy, D. and Thodos, G. Thermal Conductivity of Gases. *I&EC Fund.*, 7, 529-35 (1968).
- Roy, D. and Thodos, G. Thermal Conductivity of Gases. *I&EC Fund.*, 9, 71-8 (1970.)
- Santodanato, J., Bush, C., Howard, K., DelFavero, D., Miles, PC., Merrick, ET., Smith, LK., and Travers, L. TSCATS: A Database for Chemical and Subject Indexing of Health and Environmental Studies Submitted Under the Toxic Substances Control Act. *Env. Tox. Chem.*, 6, 921-7 (1987).
- Smith, ND. Correspondence. Environmental Protection Agency, Air and Energy Engineering Research Laboratory, Research Triangle Park, NC, November 24 (1993).
- Stein, SE. and Brown, RL. Estimation of Normal Boiling Points from Group Contributions. *J. Chem. Inf. Compu. Sci.*, 34, 581-7 (1994).
- Suehla, RA. Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures. U.S. Department of Commerce, National Technical Information Service. Springfield, VA. N63-22862 (1962).
- Suh, KW. Foamed Plastics in Kirk-Othmer Encyclopedia of Chemical Technology. Fourth Edition. John Wiley and Sons, New York, NY. A11: 729-83 (1994).
- Taverna, M. and Corradi, P. Meeting the Safety Challenges of Making Pentane-Blown Foams. *Modern Plastics*, November, 65-69 (1994).
- Tomlinson, D., English, G., and Bazzo, W. An Effective Strategy to Eliminate CFCs in Refrigerator Insulation. *Proceedings of the Polyurethanes World Congress, 1993*. Technomic Publishing Co., Lancaster, PA, 2-4 (1993).
- Visscher, PT., Culbertson, CW., and Oremland, RS. Degradation of Trifluoroacetate in Oxic and Anoxic Sediments. *Nature*, 369 (6483), 729 (1994).

Volkert, O. Cyclopentane-Blown Rigid Foams for Refrigerators. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 29-32 (1993).

Walker, GW., Tomlinson, D., English, G., and Bazzo, W. An Effective Strategy to Eliminate CFCs in Refrigerator Insulation. Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 2-9 (1993).

Wallington, TJ. and Schneider, WF. The Stratospheric Fate of CF_3OH . Environ. Sci. Technol., 28(6), 1198-1200 (1994).

Wallington, TJ., Schneider, WF., Worsnop, DR., Nielsen, OJ., Sehested, J., Debruyne, WJ., and Shorter, JA. The Environmental Impact of CFC Replacements - HFCs and HCFCs. Environ. Sci. Technol. 28, 320A-326A (1994).

Wiederman, RE., Heilig, GG., and Hoppe, EM. Aging Characteristics of PUR Rigid Foams with Alternative Blowing Agents. Proceedings of the Polyurethanes World Congress, 1991. Technomic Publishing Co., Lancaster, PA, 408-11 (1991).

Wuebbles, DJ. and Edmonds, J. Primer on Greenhouse Gases. Lewis Publishers, Chelsea, MI. (1991).

Yalkowsky, S.H., Valvani, S.C., Kuo, W., and Dannenfelser, R. Arizona Database of Aqueous Solubility (1987).

Yu-Halada, LC. and Reichel, CJ. Zero-ODP Rigid Insulation Foams Prepared with HFAs, Proceedings of the Polyurethanes World Congress, 1993. Technomic Publishing Co., Lancaster, PA, 383-85 (1993).

Zhang, Z., Padmaja, S., Saini, RD., Huie, RE., and Kurylo, MJ. Reactions of Hydroxyl Radicals with Several Hydrofluorocarbons: The Temperature Dependencies of the Rate Constants for $\text{CHF}_2\text{CF}_2\text{CH}_2\text{F}$ (HFC-245ca), $\text{CF}_3\text{CHFCHF}_2$ (HFC-236ea), $\text{CF}_3\text{CHF}_2\text{CF}_3$ (HFC227ea), and $\text{CF}_3\text{CH}_2\text{CH}_2\text{CF}_3$ (HFC-356ffa). J. Phys. Chem., 98, 4312-5 (1994).